

# **Protocol for the Application of the CALPUFF Model for Analyses of Best Available Retrofit Technology (BART)**

**December 22, 2005**

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**Visibility Improvement State and Tribal Association  
of the Southeast (VISTAS)**

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## SUMMARY

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This Protocol for the Application of the CALPUFF Model for Analyses of Best Available Retrofit Technology (BART) for the VISTAS Regional Planning Organization (RPO) describes common procedures for carrying out air quality modeling to support BART determinations that are consistent with guidelines of the U.S. Environmental Protection Agency in 40 CFR Part 51 Appendix W and Appendix Y. The Protocol is intended to serve as the basis for a common understanding among the organizations that will be performing BART analyses or reviewing the BART modeling results in the VISTAS region.

### Background

Best Available Retrofit Technology is required for any BART-eligible source that “emits any air pollutant which may reasonably be anticipated to cause or contribute to any impairment of visibility” in any mandatory Class I federal area. According to 40 CFR Part 51 Appendix Y, “*You can use dispersion modeling to determine that an individual source cannot reasonably be anticipated to cause or contribute to visibility impairment in a Class I area and thus is not subject to BART.*” In the “individual source attribution approach,” a BART-eligible source that is responsible for a 1.0 deciview (dv) change or more is considered to “cause” visibility impairment. A BART-eligible source that is responsible for a 0.5 dv change or more is considered to “contribute” to visibility impairment in a Class I area. Any source determined to cause or contribute to visibility impairment in any Class I area is subject to BART.

The member states of the VISTAS RPO agreed to develop a common BART Modeling Protocol to guide them, their sources, and reviewers in the BART determination and review effort. The Protocol has been in preparation within VISTAS since January 2005. The original authors are Pat Brewer, VISTAS Technical Coordinator, and Ivar Tombach, VISTAS Technical Advisor. The VISTAS state BART contacts, particularly Tom Rogers, FL, Chris Arrington, WV, Leigh Bacon, AL, and Michael Kiss, VA, have directed and extensively reviewed the Protocol. The Protocol was enhanced and completed with the assistance of Joseph Scire, Christelle Escoffier-Czaja and Jelena Popovic of Earth Tech, Inc. and it has received extensive contributions and review from the VISTAS federal partners: Federal Land Managers and US EPA. The VISTAS RPO held a meeting on September 21, 2005 in Research Triangle Park, NC to discuss the Protocol with participants before starting a public comment period. The Protocol underwent formal external review during the period between September 26, 2005 and October 31, 2005. Numerous comments were received. All comments were carefully considered and discussed with VISTAS participants and federal partners. VISTAS gratefully acknowledges the very useful contributions of those that provided comments. On November 1<sup>st</sup>, 2005 VISTAS held another meeting with its participants in Nashville, TN to present and discuss the comments being considered for inclusion in the Protocol. No formal document will be prepared to address all the comments received on the Protocol.

## Objectives

The objectives of the Protocol (discussed in Chapter 1) are to provide:

- A consistent approach to determine if a source is subject to BART
- A consistent model (CALPUFF) and modeling guidelines for BART determinations
- Clearly delineated modeling steps
- A common CALPUFF configuration
- Guidance for site-specific modeling
- Common expectations for reporting model results

The Protocol is not intended to define the engineering analyses required by the US EPA's BART Guidance, nor address model alternatives to the CALPUFF model, nor address emissions trading.

Chapter 2 is intended to provide summary background on EPA's guidance for BART modeling. The CALPUFF model system is reviewed in Chapter 3, while specific recommendations for applying the CALPUFF model for BART purposes appear in Chapter 4. Chapter 5 describes the specific information that should be included in site-specific protocols. Chapter 6 describes the quality assurance requirements for BART analyses in the VISTAS RPO.

## Recommendations

The major recommendations for VISTAS BART modeling included in this Protocol are:

### ***I. Process***

Follow the BART process steps discussed in Chapter 2:

1. Identify BART eligible sources
2. Identify which pollutants have greater than *de minimis* emission levels
3. Identify sources that are subject to BART
4. Identify baseline visibility impact of each BART source
5. Identify feasible controls and emission changes
6. Identify the change in visibility impact for each candidate BART control option
7. Compare the visibility improvement of BART control options to other statutory factors in the engineering analysis

## II. CALPUFF Model Configuration

Use the CALPUFF dispersion modeling system, as described in Chapter 4, to determine if a single source is subject to BART. VISTAS will use CALPUFF Version 5.754 and CALMET Version 5.7. These versions contain enhancements funded by the Minerals Management Service (MMS) and VISTAS. They were developed by Earth Tech, Inc. and are maintained on the CALPUFF website ([www.src.com](http://www.src.com)) for public access.

VISTAS is making publicly available 12-km CALMET output files for the entire VISTAS modeling domain (eastern United States) and intends to also provide CALMET output files for five 4-km grid subdomains covering the VISTAS states and VISTAS Class I areas. To create the CALMET input files, Earth Tech used the MM5 databases developed by EPA for 2001, VISTAS for 2002, and Midwest RPO for 2003. For the 12 km grid large domain covering the entire VISTAS region, Earth Tech used the No-Obs setting (i.e., did not include additional surface and upper air observations beyond those incorporated in the MM5 calculations). For finer resolution subdomains (4 km grid or less), available surface and upper air observations will be used in addition to MM5 meteorological model outputs. The specific model settings will be provided with the CALMET files and via the CALPUFF website so that users can review or replicate the work.

For CALPUFF modeling, source emissions should be defined using the maximum 24-hour actual emission rate during normal operation for the most recent 3 or 5 years. If maximum 24-hr actual emissions are not available, continuous emissions data, permit allowable emissions, potential emissions, and emissions factors from AP-42 source profiles may be used as available.

Key points from comments received on the specific CALPUFF, CALPOST, and POSTUTIL configurations are highlighted below.

- After running CALPUFF for an individual facility, repartition NO<sub>3</sub> in POSTUTIL.<sup>1</sup>
- Use ozone data from non-urban monitors as the background ozone input.
- Use the Pasquill-Gifford dispersion method.<sup>2</sup>

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<sup>1</sup> The original intent, as expressed in the Final VISTAS BART Modeling Protocol (22 December 2005) was to use CMAQ-derived background data for SO<sub>2</sub>, NO<sub>3</sub> and NH<sub>3</sub> in POSTUTIL. After extensive discussion with the EPA and FLMs in early 2006, EPA did not approve the recommended approach so background gaseous concentrations from CMAQ 2002 modeling will not be provided by VISTAS for use in POSTUTIL. Rather the standard default NH<sub>3</sub> concentrations specified on page 14 of the IWAQM Phase 2 report (IWAQM, 1998) will be used.

<sup>2</sup> The Final VISTAS BART Modeling Protocol (Dec. 22, 2005) recommended using turbulence-based AERMOD dispersion methods, citing EPA's *Revision to the Guideline on Air Quality Models: Adoption of a Preferred General Purpose (Flat and Complex Terrain) Dispersion Model and Other Revisions; Final Rule*. 70 FR 68218-68261. 9 November 2005. Subsequently, EPA Region IV notified the VISTAS states that using turbulence-

- In CALPOST, use Method 6 with monthly average RH for calculating extinction, as recommended by the EPA.
- Use EPA default calculations of light extinction under current and natural background conditions. In addition to the default assumptions, a source may choose to also calculate visibility using the recently revised IMPROVE algorithm described by Pitchford, et al., (2005).

Provide results in tables as illustrated in Chapter 4 that describe, for each source:

- Number of receptors within a single Class I area with impact > 0.5 dv
- Number of days at all receptors in the Class I area with impact > 0.5 dv
- Number of Class I areas with impacts > 0.5 dv

### ***III. CALPUFF Application for BART***

For determining if a BART-eligible source is subject to BART CALPUFF modeling, use a two-tier approach. For the initial exemption modeling use CALPUFF with 12-km grid CALMET. For finer resolution of meteorological fields, use CALPUFF with CALMET of 4-km or smaller grid size.

VISTAS States are accepting EPA guidance that the threshold value to establish that a source contributes to visibility impairment is 0.5 deciview.

VISTAS States are using emissions (tons per year) divided by distance (km) from a Class I area boundary (Q/d) as a presumptive indicator that a BART-eligible source is subject to BART. If Q/d for SO<sub>2</sub> is greater than 10 for 2002 actual annual emissions, then the State presumes that the source is subject to BART and no exemption modeling will be performed using VISTAS funds. If the source agrees with this presumption, then the source can proceed to the BART determination using CALPUFF to evaluate impacts of control options and perform the engineering analyses. If a source disagrees, the source may perform fine grid modeling to determine if its impact is <0.5 dv.

For sources with Q/d less than or equal to 10, VISTAS intends to fund TRC Environmental Corp.<sup>3</sup> to assist States with the initial CALPUFF exemption modeling. Each State will prioritize which sources will be offered modeling by VISTAS. Modeling of these sources will be conducted in priority order to first accommodate States with nearer term timing constraints in their SIP development process. To conserve VISTAS resources, modeling will begin with sources at lower Q/d values and continue with sources with higher Q/d values until a Q/d value

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based dispersion methods would be considered a non-guideline application of CALPUFF. Thus this Protocol has been revised to indicate Pasquill-Gifford dispersion coefficients should be used.

<sup>3</sup> In April 2006, Earth Tech's CALPUFF modeling staff became part of TRC Environmental Corporation. References to Earth Tech and to TRC in this protocol refer to the same technical staff, just at different times.

that consistently results in a greater than 0.5 dv impact is identified. Chapter 4 addresses the number of VISTAS sources eligible for BART based on Q/d analysis.

Note that VISTAS does not propose to use Q/d to exempt BART-eligible sources, but only to prioritize sources for modeling purposes. Thus this application is consistent with EPA guidance not to use Q/d for exemption purposes.

For the 12-km initial modeling exemption test, compare the highest single 24-hour average value across all receptors in the Class I area to the threshold value of 0.5 dv. If the highest 24-hr average value is below 0.5 dv at all Class I areas, then the source is not subject to BART. If the highest 24-hr average value is greater than 0.5 dv, then the source may choose to perform finer grid modeling for exemption purposes or may accept determination that the source is subject to BART and proceed to establish visibility impacts prior to and after BART controls. If using the single highest 24-hr average value proves, after initial 12-km grid CALPUFF modeling, to be too conservative a screening level, VISTAS may allow some exceedances of the threshold value for exemption purposes, up to no more than the 98<sup>th</sup> percentile value.

The 12-km modeling results can be used to focus finer grid modeling for exemption purposes on only those Class I areas where impacts greater than 0.5 dv were projected in the 12-km modeling.

For finer grid (4 km or less) analyses, use the 98<sup>th</sup> percentile impact value for the 24-hr average. Use either the 8<sup>th</sup> highest day in each year or the 22<sup>nd</sup> highest day in the 3-year period, whichever is more conservative, for comparison to the exemption threshold.

Use the same model assumptions for pre-BART visibility impact and for BART control options modeling: establish baseline visibility from the pre-BART run; change one control at a time; and evaluate the change in visibility impact, i.e. the delta-deciview. Note that “no control” may constitute BART.

Visibility impact is one of the five factors considered in the engineering analysis required under the USEPA BART guideline. If a source accepts to institute the most stringent control, the engineering analyses are not required.

This common VISTAS Protocol consistently recommends conservative assumptions. Individual States ultimately have responsibility to determine which, if any, BART controls are recommended in their State Implementation Plans (SIPs).



# **1. INTRODUCTION AND PROTOCOL OBJECTIVES**

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## **1.1 Background**

Under regional haze regulations, the Environmental Protection Agency (EPA) has issued final guidelines dated July 6, 2005 for Best Available Retrofit Technology (BART) determinations (70 FR 39104-39172). The regional haze rule includes a requirement for BART for certain large stationary sources. Sources are BART-eligible if they meet three criteria including potential emissions of at least 250 tons per year of a visibility-impairing pollutant, were put in place between August 7, 1962 and August 7, 1977, and fall within one of the 26 listed source categories in the guidance. A BART engineering evaluation using five statutory factors -- 1) existing controls; 2) cost; 3) energy and non-air environmental impacts; 4) remaining useful life of the source; 5) degree of visibility improvement expected from the application of controls -- is required for any BART-eligible source that can be reasonably expected to cause or contribute to impairment of visibility in any of the 156 federal parks and wilderness (Class I) areas protected under the regional haze rule. (Note that, depending on the five factors, the evaluation may result in no control.) Air quality modeling is an important tool available to the States to determine whether a source can be reasonably expected to contribute to visibility impairment in a Class I area.

Throughout this document the term “BART-eligible emission unit” is defined as any single emission unit that meets the criteria described above. A “BART-eligible source” is defined as the total of all BART-eligible emission units at a single facility. If a source has several emission units, only those that meet the BART-eligible criteria are included in the definition “BART-eligible source”.

One of the listed categories is steam electric plants of more than 250 million BTU/hr heat input. To determine if such a plant has greater than 250 million BTU/hr heat input and is potentially subject to BART, the boiler capacities of all electric generating units (EGUs) should be added together regardless of construction date. In this category, electric generating sources greater than 750 MW have presumptive SO<sub>2</sub> and NO<sub>x</sub> emission limits. States may presume the same limits for EGU sources between 250-750 MW. However, units at those sources constructed after the BART-eligibility dates are not subject to a BART engineering evaluation. EPA, in the Clean Air Interstate Rule (CAIR), determined that an EGU participating in the CAIR trading program satisfies the BART requirements for SO<sub>2</sub> and NO<sub>x</sub>. VISTAS states are tentatively accepting this guidance. CAIR does not cover PM so EGUs would still need to evaluate impacts of PM if PM emissions are above *de minimis* values.

As illustrated in Table 1-1, as of December 5, 2005, VISTAS States had identified a total of 274 BART-eligible sources that fall into 20 of the 26 BART source categories. Of the 274 sources with BART-eligible units, 84 sources are utility EGUs and 190 are non-EGU industrial sources. (Note that these numbers are not final and are subject to slight adjustments and refinements.) No BART sources are located on Tribal lands.

**Table 1-1. VISTAS BART Eligible Sources** (not updated since December 2005)

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<b>State</b>	<b>Total Number of Sources</b>	<b>EGU Sources</b>	<b>Non-EGU Sources</b>
AL	48	8	40
FL	50	23	27
GA	24	10	14
KY	29	12	17
MS	18	8	10
NC	16	5	11
SC	31	6	25
TN	13	2	11
VA	18	3	15
WV	26	7	19
<b>Total</b>	<b>273</b>	<b>84</b>	<b>189</b>

## **1.2 Objective of this Protocol**

The objective of this VISTAS' BART Modeling Protocol is to describe common procedures for air quality modeling to support BART determinations that are consistent with the EPA guidelines. The protocol will serve as the basis for establishing a common understanding among the organizations who will be performing the BART analyses or reviewing the BART modeling results, including VISTAS State and Local air regulatory agencies, EPA, Federal Land Managers (FLMs), source operators, and contractors for the sources. This final protocol incorporates EPA final guidance and comments that were received on VISTAS' draft protocol<sup>4</sup> and provides additional description of modeling procedures. The original final protocol of 22 December 2005 has been revised since then to clarify items, resolve technical issues, and reflect decisions by the EPA and FLMs. This document is the third revision.

The VISTAS States have accepted EPA's guidance to use the CALPUFF modeling system to comply with the BART modeling requirements of the regional haze rule. A BART-eligible source will be required to submit a site-specific modeling protocol to the State for review and approval prior to performing CALPUFF modeling. States will consult with FLMs and the EPA when evaluating the site-specific BART protocols. The site-specific protocol will include the

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<sup>4</sup> *Draft Protocol for the Application of the CALPUFF Model for Analyses of Best Available Retrofit Technology (BART)*. VISTAS, March 22, 2005 and September 20, 2005.

source-specific data on source location, stack parameters, and emissions. The methods of the VISTAS common modeling protocol will be followed in the site-specific protocol unless the source proposes to the State, and the State approves, alternative methods or assumptions.

Each VISTAS State or Local agency retains responsibility for the specific procedures and processes it will follow in working with the BART sources under its jurisdiction, the FLMs, EPA, and public to determine BART controls for sources in the State. Nothing in the VISTAS process replaces States' responsibility to determine BART controls.

The remainder of this document describes the CALPUFF modeling system and the application of CALPUFF to two situations:

- Air quality modeling to determine whether a BART-eligible source is “subject to BART” and therefore the BART analysis process must be applied to its operations.
- Air quality modeling of emissions from sources that have been found to be subject to BART, to evaluate regional haze benefits of alternative control options and to document the benefits of the preferred option.

Chapters 2 and 3 of this document are intended to provide background information on EPA's guidance for BART analysis modeling and on the CALPUFF modeling system. Subsequent chapters include more specific recommendations. Chapter 2 of this document reviews EPA's guidance for regional haze BART analysis modeling, as outlined in the 6 July 2005 Federal Register notice. The CALPUFF model is the preferred model recommended by the EPA for BART modeling analyses and its characteristics and limitations are discussed in Chapter 3. The specific steps to determine whether a BART-eligible source is subject to BART and to evaluate BART controls are described in Chapter 4. The procedures include initial modeling of BART-eligible sources using CALPUFF run in a conservative mode with regional meteorological datasets. For sources determined to be subject to BART based on these first modeling analyses, further finer grid CALPUFF analyses would be performed. The model configuration for the common modeling protocol is described in Chapter 4. Details of the source-specific protocol are described in Chapter 5. A quality assurance plan is outlined in Chapter 6.

EPA's guidance allows for the use of appropriate alternative models, however VISTAS will not develop a protocol for alternative models. This protocol focuses on guidance for the application of the preferred CALPUFF modeling approach. If a source wants to use an alternative model in its BART demonstration, the source will need to submit a detailed written justification to the State for review and approval. The State will provide the documentation to the EPA and Federal Land Managers for their review.

Also, this protocol does not address a preferred modeling approach to demonstrate the effectiveness of an optional emissions cap and trade program. Such a cap and trade program is not required, but can be implemented in lieu of BART if desired by the VISTAS States. VISTAS

States are not pursuing a regional trading alternative under the proposed EPA trading guidance (70 FR 44154-44175) that is to be promulgated in 2006.

## 2. REVIEW OF EPA'S GUIDANCE FOR BART MODELING

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The final guidance for regional haze BART determinations was published in the Federal Register on 6 July 2005 (70 FR 39104 to 39172). It prescribes the modeling approaches that are to be used for various stages of the BART analysis process.

This chapter provides a summary of EPA's guidance for BART modeling. It is not intended to provide a comprehensive review of the guidance. Nor does this chapter address specific recommendations for VISTAS' approach to CALPUFF BART modeling. Those recommendations appear in Chapter 4.

### 2.1 Overview of the Regional Haze BART Process

The process of establishing BART emission limitations consists of four steps:

1) Identify whether a source is "BART-eligible" based on its source category, when it was put in service, and the magnitude of its emissions of one or more "visibility-impairing" air pollutants. The BART guidelines list 26 source categories of stationary sources that are BART-eligible. Sources must have been put in service between August 7, 1962 and August 7, 1977 in order to be BART-eligible. Finally, a source is eligible for BART if potential emissions of visibility-impairing air pollutants are greater than 250 tons per year. Qualifying pollutants include primary particulate matter (PM<sub>10</sub>) and gaseous precursors to secondary fine particulate matter, such as SO<sub>2</sub> and NO<sub>x</sub>. Whether ammonia or volatile organic compounds (VOCs) should be included as visibility-impairing pollutants for BART eligibility is left for the States to determine on a case-by-case basis. The guidance states that high molecular weight VOCs with 25 or more carbon atoms and low vapor pressure should be considered as primary PM<sub>2.5</sub> emissions and not VOCs for BART purposes.

(Note: If the source is subject to BART because one visibility impairing pollutant has potential emissions > 250 TPY, the State may determine that other visibility impairing pollutants are not subject to BART if their potential emissions are less than the *de minimis* levels (40 TPY for SO<sub>2</sub> and NO<sub>x</sub> and 15 TPY of PM<sub>10</sub> or PM<sub>2.5</sub>. This assumes that the other BART-eligibility criteria are met.)

2) Determine whether a BART-eligible source can be excluded from BART controls by demonstrating that the source cannot be reasonably expected to cause or contribute to visibility impairment in a Class I area. The preferred approach is an assessment with an air quality model such as CALPUFF or other appropriate model followed by comparison of the estimated 24-hr visibility impacts against a threshold above estimated natural conditions to be determined by the States.<sup>5</sup> The threshold to determine whether a single source "causes" visibility impairment is set at

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<sup>5</sup> A recent draft settlement agreement with the EPA (to be published in the *Federal Register* for public comment) provides that a State has the discretion to decide whether annual average or 20% best natural conditions are to be used as the reference. This ruling resolves an ambiguity in EPA's BART guidance, where the BART guideline

1.0 deciview change from natural conditions over a 24-hour averaging period in the final BART rule (70 FR 39118). The guidance also states that the proposed threshold at which a source may “contribute” to visibility impairment should not be higher than 0.5 deciviews although, depending on factors affecting a specific Class I area, it may be set lower than 0.5 deciviews. The test against the threshold is “driven” by the contribution level, since if a source “causes”, by definition it “contributes”.

EPA recommends that the 98<sup>th</sup> percentile value from the modeling be compared to the contribution threshold of 0.5 deciviews (or a lower level set by a State) to determine if a source does not contribute to visibility impairment and therefore is not subject to BART. Whether or not the 98<sup>th</sup> percentile value exceeds the threshold must be determined at each Class I area. Over an annual period, this implies the 8<sup>th</sup> highest 24-hr value at a particular Class I area is compared to the contribution threshold. Over a 3-year modeling period, the 98<sup>th</sup> percentile value may be interpreted as the highest of the three annual 98<sup>th</sup> percentile values at a particular Class I area or the 22<sup>nd</sup> highest value in the combined three year record, whichever is more conservative.

Alternatively, States have the option of considering that all BART-eligible sources within the State are subject to BART and skipping the initial impact analysis. In rare cases, a State might be able to do exactly the opposite, and use regional modeling to conclude that all BART-eligible sources in the State do not cumulatively contribute to “measurable” visibility impairment in any Class I areas. Also, the States have an option to exempt individual sources based on model plant analysis conducted by EPA in finalizing the BART rule. Under this option, sources with potential emissions of SO<sub>2</sub> plus NO<sub>x</sub> of less than 500 tons and a distance from any Class I area greater than 50 kilometers or sources with SO<sub>2</sub> plus NO<sub>x</sub> potential emissions of less than 1000 tons and a distance from any Class I area greater than 100 kilometers can be exempted. PM emissions are not specifically addressed in the model plant analysis, but subsequent discussions with EPA staff indicate that PM may be considered along with SO<sub>2</sub> and NO<sub>x</sub>, so that a plant could be exempted if the combined potential emissions of SO<sub>2</sub>, NO<sub>x</sub>, plus PM meet the criteria above.

3) Determine BART controls for the source by considering various control options and selecting the “best” alternative, taking into consideration:

- a) Any pollution control equipment in use at the source (which affects the availability of options and their impacts),
- b) The costs of compliance with control options,
- c) The remaining useful life of the facility,
- d) The energy and non air-quality environmental impacts of compliance, and

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text says “natural conditions” at 70 FR 39162, col. 3, while the preamble to the BART rule says “natural visibility baseline for the 20% best visibility days” at 70 FR 39125, col. 1.

- e) The degree of improvement in visibility that may reasonably be anticipated to result from the use of such technology.

Note that if a source agrees to apply the most stringent controls available to BART-eligible units, the BART analysis is essentially complete and no further analysis is necessary (70 FR 39165).

- 4) Incorporate the BART determination into the State Implementation Plan for Regional Haze, which is due by December 2007.

Instead of applying BART on a source-by-source basis, a State (or a group of States) has the option of implementing an emissions trading program that is designed to achieve regional haze improvements that are greater than the visibility improvements that could be expected from BART. If the geographic distributions of emissions under the two approaches are similar, determining whether trading is “better than BART” may be possible by simply comparing emissions expected under the trading program against the emissions that could be expected if BART was applied to eligible sources. If the geographic distributions of emissions are likely to be different, however, air quality modeling comparing the expected improvements in visibility from the trading program and from BART would be required. (See the proposed BART Alternative rule, at 70 FR 44160.) EPA suggests that regional modeling using a photochemical grid model may be more appropriate than CALPUFF for this purpose.

Note that EPA has indicated in the BART rule (70 FR 39138-39139) that emissions reductions under the Clean Air Interstate Rule (CAIR) meet the BART requirement for SO<sub>2</sub> and NO<sub>x</sub> control for those EGUs subject to BART. However, PM emissions from EGUs are not addressed by CAIR and therefore a BART analysis may still be required for PM.

## **2.2 Model Recommendations for the BART Analysis**

To evaluate the visibility impacts of a BART-eligible source at Class I areas beyond 50 km from the source, the EPA guidance recommends the use of the CALPUFF model as “the best regulatory modeling application currently available for predicting a single source’s contribution to visibility impairment” (70 FR 39162). The use of another “appropriate model” is allowed although the EPA prefers the use of CALPUFF. If a source wants to use an alternative model, the source needs to submit a written justification and source-specific modeling protocol to its State for review and approval. As part of the consultation process, the State will provide documentation to EPA and FLM.

For modeling the impact of a source closer than 50 km to a Class I area, EPA’s BART guidance recommends that expert modeling judgment be used, “giving consideration to both CALPUFF and other methods.” The PLUVUE-II plume visibility model is mentioned as a possible model to consider instead of CALPUFF for a source within less than 50 km of a Class I area.

The EPA guidance notes that “regional scale photochemical grid models may have merit, but such models have been designed to assess cumulative impacts, not impacts from individual sources” and

they are “very resource intensive and time consuming relative to CALPUFF”, but States may consider their use for SIP development in the future as they may be adapted and “demonstrated to be appropriate for single source applications” (70 FR 39123). Photochemical grid models may be more appropriate for cumulative modeling options such as in the determination of the aggregate contribution of all-BART-eligible sources to visibility impairment, but such use should involve consultation with the appropriate EPA Regional Office (70 FR 39163).

According to the BART guidance, a modeling protocol should be submitted for all modeling demonstrations regardless of the distance from the BART-eligible source to the Class I area. EPA’s role in the development of the protocol is only advisory as the “States better understand the BART-eligible source configurations” and factors affecting their particular Class I areas (70 FR 39126).

In the BART modeling analyses the EPA recommends that the State use the highest 24-hour average actual emission rate for the most recent three to five-year period of record. Emissions on days influenced by periods of start-up, shutdown and malfunction are not to be considered in determining the appropriate emission rates. (70 FR 39129).

If a source is found to be subject to BART, CALPUFF or another appropriate model should be used to evaluate the improvement in visibility resulting from the application of BART controls. Visibility improvements may be evaluated on a pollutant-specific basis in the BART determination (70 FR 39129).

For evaluating the improvement in visibility resulting from the application of BART, the EPA guidelines state that States are “encouraged to account for the magnitude, frequency, and duration of the contributions to visibility impairment caused by the source based on the natural variability of meteorology” (70 FR 39129).

## **2.3 Performance of a Cap and Trade Program**

If a State or States elect to pursue an optional cap and trade program, they are required to demonstrate greater “reasonable progress” in reducing haze than would result if BART were applied to the same sources. In some cases, a State may simply be able to demonstrate that a trading program that achieves greater progress at reducing emissions will also achieve greater progress at reducing haze. Such would be the case if the likely geographic distribution of emissions under the trading program would not be greatly different from the distribution if BART was in place.

If the expected distribution of emissions is different under the two approaches, then “dispersion modeling” of all sources must be used to determine the difference in visibility at each impacted Class I area, in order to establish that the optional trading program will result in visibility improvements aggregated over all Class I areas that are “better than BART” (70 FR 39137-39138). The BART guidance does not specify the method to be used for this modeling. From a technical perspective, either applying CALPUFF to every source or using a regional photochemical model would satisfy the need.



A rulemaking procedure is currently underway to establish final guidance for such alternatives to BART (70 FR 44154-44175). The rule is expected to be finalized in 2006.

### 3. OVERVIEW OF THE CALPUFF MODELING SYSTEM

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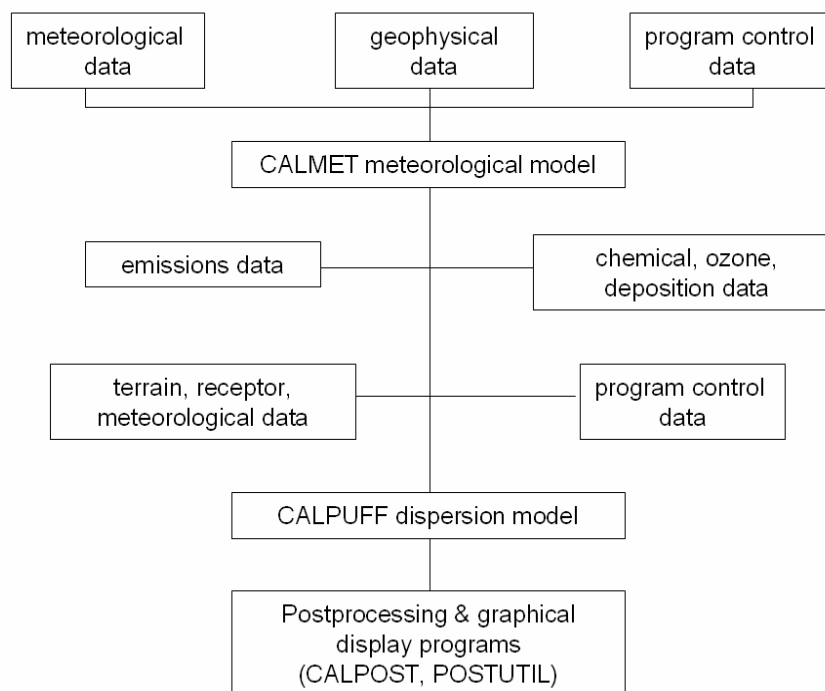
This chapter contains a general description of the CALPUFF modeling system and its capabilities and limitations. It does not include specific recommendations regarding the use of the model for BART analysis in the VISTAS region. These specific recommendations can be found in Chapter 4.

#### 3.1 Capabilities and features of CALPUFF

The CALPUFF modeling system (Scire et al., 2000a, b) is recommended as the preferred modeling approach for use in the BART analyses. CALPUFF and its meteorological model, CALMET, are designed to handle the complexities posed by the complex terrain, the large source-receptor distances, chemical transformation and deposition, and other issues related to Class I visibility impacts. The CALPUFF modeling system has been adopted by the EPA as a *Guideline Model* for source-receptor distances greater than 50 km, and for use on a case-by-case basis in complex flow situations for shorter distances (68 FR 18440-18482). CALPUFF is recommended for Class I impact assessments by the Federal Land Managers Workgroup (FLAG 2000) and the Interagency Workgroup on Air Quality Modeling (IWAQM) (EPA 1998). The final BART guidance recommends CALPUFF as “the best modeling application available for predicting a single source’s contribution to visibility impairment” (70 FR 39122). As a result of these recommendations, the VISTAS modeling protocol is based on the use of CALPUFF for its BART determinations.

The main components of the CALPUFF modeling system are shown in Figure 3-1. CALMET is a diagnostic meteorological model that is used to drive the CALPUFF dispersion model. It produces three-dimensional wind and temperature fields and two-dimensional fields of mixing heights and other meteorological fields. It contains slope flow effects, terrain channeling, and kinematic effects of terrain. CALMET includes special algorithms for treating the overwater boundary layer and coastal interaction effects. CALMET can use meteorological observational data and/or three-dimensional output from prognostic numerical meteorological models such as MM5 (Grell et al., 1995) or RUC (Benjamin et al., 2004) in the developments of its fine-scale meteorological fields.

CALPUFF is a non-steady-state Lagrangian puff transport and dispersion model that advects Gaussian puffs of multiple pollutants from modeled sources. CALPUFF’s algorithms have been designed to be applicable on spatial scales from a few tens of meters to hundreds of kilometers from a source. It includes algorithms for near-field effects such as building downwash, stack tip downwash and transitional plume rise as well as processes important in the far-field such as chemical transformation, wet deposition, and dry deposition. CALPUFF contains an option to allow puff splitting in the horizontal and vertical directions, which extends the distance range of the model. The primary outputs from CALPUFF are hourly concentrations and hourly deposition fluxes evaluated at user-specified receptor locations.



**Figure 3-1. CALPUFF modeling system components.**

A set of postprocessing programs associated with CALPUFF computes visibility effects and allows cumulative source impacts to be assessed, including potential non-linear effects of ammonia limitation on nitrate formation. The CALPOST postprocessor contains several options for computing change in extinction and deciviews for visibility assessments. The POSTUTIL postprocessor includes options for summing contributions of individual sources or groups of sources to assess cumulative impacts. POSTUTIL also contains CALPUFF's nitric acid-nitrate chemical equilibrium module, which allows the cumulative effects of ammonia consumption by background sources to be assessed in the postprocessor. In addition, the combination of CALPUFF and POSTUTIL allows the effects of source emissions of ammonia to be incrementally added to background ammonia levels when determining nitrate formation.

The rest of this chapter summarizes the capabilities and features of the CALPUFF modeling components in more detail.

### 3.1.1 Major Features of CALMET

The CALMET meteorological model consists of a diagnostic wind field module and micrometeorological modules for overwater and overland boundary layers. When modeling a large geographical area, as would be necessary for the regional VISTAS domain, the user has the option to use a Lambert Conformal Projection coordinate system to account for Earth's curvature.

The major features and options of the meteorological model are summarized in Table 3-1. The techniques used in the CALMET model are briefly described below.

**Table 3-1. Major Features of the CALMET Meteorological Model**

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- **Boundary Layer Modules of CALMET**
  - Overland Boundary Layer - Energy Balance Method
  - Overwater Boundary Layer - Profile Method
    - COARE algorithm
    - OCD-based method
  - Produces Gridded Fields of:
    - Surface Friction Velocity
    - Convective Velocity Scale
    - Monin-Obukhov Length
    - Mixing Height
    - PGT Stability Class
    - Air Temperature (3-D)
    - Precipitation Rate
- **Diagnostic Wind Field Module of CALMET**
  - Slope Flows
  - Kinematic Terrain Effects
  - Terrain Blocking Effects
  - Divergence Minimization
  - Produces Gridded Fields of U, V, W Wind Components
  - Inputs Include Domain-Scale Winds, Observations, and (optionally) Coarse-Grid Prognostic Model Winds
  - Lambert Conformal Projection Capability

#### ***CALMET Boundary Layer Models***

The CALMET model contains two boundary layer models for application to overland and overwater grid cells.

*Overland Boundary Layer Model:* Over land surfaces, the energy balance method of Holtslag and van Ulden (1983) is used to compute hourly gridded fields of the sensible heat flux, surface

friction velocity, Monin-Obukhov length, and convective velocity scale. Mixing heights are determined from the computed hourly surface heat fluxes and observed temperature soundings using a modified Carson (1973) method based on Maul (1980). The model also determines gridded fields of Pasquill-Gifford-Turner (PGT) stability class and hourly precipitation rates.

*Overwater Boundary Layer Model:* The aerodynamic and thermal properties of water surfaces suggest that a different method is best suited for calculating the boundary layer parameters in the marine environment. A profile technique, using air-sea temperature differences, is used in CALMET to compute the micro-meteorological parameters in the marine boundary layer. The version of CALMET being used by VISTAS contains improvements in the overwater boundary layer parameterizations (Fairall et al., 2003) based on the Coupled Ocean Atmosphere Response Experiment (COARE) and enhancements in the calculation of overwater mixed layer heights (Batchvarova and Gryning, 1991, 1994). Further details and the results of an evaluation of the model containing these enhancements are described in Scire et al. (2005). An upwind-looking spatial averaging scheme is optionally applied to the mixing heights and three-dimensional temperature fields in order to account for important advective effects.

### ***Diagnostic Wind Field Module***

The diagnostic wind field module uses a two-step approach to the computation of the wind fields (Douglas and Kessler, 1988). In the first step, an initial-guess wind field is adjusted for kinematic effects of terrain, slope flows, and terrain blocking effects to produce a Step 1 wind field. Gridded MM5 can be used to define the initial guess field. The second step consists of an objective analysis procedure to introduce observational data into the Step 1 wind field to produce a final wind field.

***Step 1 Wind Field.*** Development of the Step 1 wind field begins with the initial guess field defined by the MM5 prognostic meteorological model. Normally, the CALMET computational domain is specified to be at finer grid resolution than the MM5 dataset used to initialize the initial guess field. For example, 36-km MM5 data available for VISTAS modeling may be used to develop the initial guess field on a 12-km or even a 1-km CALMET grid. The Step 1 algorithms in CALMET described below apply terrain adjustments to the initial guess field on the fine-scale CALMET grid. Thus, the CALMET winds are adjusted to respond to fine-scale terrain features not necessarily seen by the coarser scale MM5 model.

*Kinematic Effects of Terrain:* The approach of Liu and Yocke (1980) is used to evaluate the effects of the terrain on the wind field. The initial guess field winds are used to compute a terrain-forced vertical velocity, subject to an exponential, stability-dependent decay function. The effects of terrain on the horizontal wind components are evaluated by applying a divergence-minimization scheme to the initial guess wind field. The divergence minimization scheme is applied iteratively until the three-dimensional divergence is less than a threshold value.

*Slope Flows:* The original slope flow algorithm in CALMET has been upgraded (Scire and Robe, 1997) based on the shooting flow algorithm of Mahrt (1982). This scheme includes both

advective-gravity and equilibrium flow regimes. At night, the slope flow model parameterizes the flow down the sides of the valley walls into the floor of the valley, and during the day, upslope flows are parameterized. The magnitude of the slope flow depends on the local surface sensible heat flux and local terrain gradients. The slope flow wind components are added to the wind field adjusted for kinematic effects.

*Blocking Effects:* The thermodynamic blocking effects of terrain on the wind flow are parameterized in terms of the local Froude number (Allwine and Whiteman, 1985). If the Froude number at a particular grid point is less than a critical value and the wind has an uphill component, the wind direction is adjusted to be tangent to the terrain.

**Step 2 Wind Field.** The wind field resulting from the above adjustments of the initial-guess wind is the Step 1 wind field. The second step of the procedure may involve introduction of observational data into the Step 1 wind field through an objective analysis procedure. An inverse-distance squared interpolation scheme is used which weights observational data heavily in the vicinity of the observational station, while the Step 1 wind field dominates the interpolated wind field in regions with no observational data. The resulting wind field is subject to smoothing, an optional adjustment of vertical velocities based on the O'Brien (1970) method, and divergence minimization to produce a final Step 2 wind field.

The introduction of observational data in the Step 2 calculation is an option. It is also possible to run the model in “no observations” (No-Obs) mode, which involves the use only of MM5 gridded data for the initial guess field followed by fine-scale terrain adjustments by CALMET. In No-Obs mode, observational data are not used in the Step 2 calculations. The No-Obs mode is appropriate when the MM5 simulations adequately characterize the regional wind patterns and when local observations, especially surface observations, reflect local conditions on a scale smaller than that of the CALMET domain and hence their spatial representativeness may be limited. Such situations are most likely to occur when the CALMET grid scale is relatively large i.e., coarser than the scale of variation of the true wind field, which is particularly likely to occur in complex terrain or along the seashore,

### **3.1.2 Major Features of CALPUFF**

By its puff-based formulation and through the use of three-dimensional meteorological data developed by the CALMET meteorological model, CALPUFF can simulate the effects of time- and space-varying meteorological conditions on pollutant transport from sources in complex terrain. The major features and options of the CALPUFF model are summarized in Table 3-2 at the end of this subsection. Some of the technical algorithms are briefly described below.

*Complex Terrain:* The effects of complex terrain on puff transport are derived from the CALMET winds. In addition, puff-terrain interactions at gridded and discrete receptor locations are simulated using one of two algorithms that modify the puff-height (either that of ISCST3 or a general “plume path coefficient” adjustment), or an algorithm that simulates enhanced vertical dispersion derived from the weakly-stratified flow and dispersion module of the Complex Terrain

Dispersion Model (CTDMPLUS) (Perry et al., 1989). The puff-height adjustment algorithms rely on the receptor elevation (relative to the elevation at the source) and the height of the puff above the surface. The enhanced dispersion adjustment relies on the slope of the gridded terrain in the direction of transport during the time step.

*Subgrid Scale Complex Terrain (CTSG):* An optional module in CALPUFF, CTSG treats terrain features that are not resolved by the gridded terrain field, and is based on the CTDMPLUS (Perry et al., 1989). Plume impingement on subgrid-scale hills is evaluated at the CTSG subgroup of receptors using a dividing streamline height ( $H_d$ ) to determine which pollutant material is deflected around the sides of a hill (below  $H_d$ ) and which material is advected over the hill (above  $H_d$ ). The local flow (near the feature) used to define  $H_d$  is taken from the gridded CALMET fields. As in CTDMPLUS, each feature is modeled in isolation with its own set of receptors.

*Puff Sampling Functions:* A set of accurate and computationally efficient puff sampling routines is included in CALPUFF, which solve many of the computational difficulties encountered when applying a puff model to near-field releases. For near-field applications during rapidly-varying meteorological conditions, an elongated puff (slug) sampling function may be used. An integrated puff approach may be used during less demanding conditions. Both techniques reproduce continuous plume results under the appropriate steady state conditions.

*Building Downwash:* The Huber-Snyder and Schulman-Scire downwash models are both incorporated into CALPUFF. An option is provided to use either model for all stacks, or make the choice on a stack-by-stack and wind sector-by-wind sector basis. Both algorithms have been implemented in such a way as to allow the use of wind direction specific building dimensions. The PRIME building downwash model (Schulman et al., 2000) is also included in CALPUFF as an option.

*Dispersion Coefficients:* Several options are provided in CALPUFF for the computation of dispersion coefficients, including the use of turbulence measurements ( $\sigma_v$  and  $\sigma_w$ ), the use of similarity theory to estimate  $\sigma_v$  and  $\sigma_w$  from modeled surface heat and momentum fluxes, or the use of Pasquill-Gifford (PG) or McElroy-Pooler (MP) dispersion coefficients, or dispersion equations based on the CTDM. Options are provided to apply an averaging time correction or surface roughness length adjustments to the PG coefficients. In version 5.754 of CALPUFF being used by VISTAS, an option is provided to use the AERMOD turbulence profiles for determining dispersion rates, which is the most recent approach to dispersion in EPA-approved regulatory modeling. In addition, turbulence advection is included. For additional details on these features, see Scire et al. (2005).

*Overwater and Coastal Interaction Effects:* Because the CALMET meteorological model contains both overwater and overland boundary layer algorithms, the effects of water bodies on plume transport, dispersion, and deposition can be simulated with CALPUFF. The puff formulation of CALPUFF is designed to handle spatial changes in meteorological and dispersion conditions, including the abrupt changes that occur at the coastline of a major body of water.

*Dry Deposition:* A resistance model is provided in CALPUFF for the computation of dry deposition rates of gases and particulate matter as a function of geophysical parameters, meteorological conditions, and pollutant species. For particles, source-specific mass distributions may be provided for use in the resistance model. Of particular interest for BART analyses is the ability to separately model the deposition of fine particulate matter ( $< 2.5 \mu\text{m}$  diameter) from coarse particulate matter ( $2.5\text{-}10 \mu\text{m}$  diameter).

*Wind Shear Effects:* CALPUFF contains an optional puff splitting algorithm that allows vertical wind shear effects across individual puffs to be simulated. Differential rates of dispersion and transport among the “new” puffs generated from the original, well-mixed puff can substantially increase the effective rate of horizontal spread of the material. Puffs may also be split in the horizontal when the puff size becomes large relative to the grid size, to account for wind shear across the puffs.

*Wet Deposition:* An empirical scavenging coefficient approach is used in CALPUFF to compute the depletion and wet deposition fluxes due to precipitation scavenging. The scavenging coefficients are specified as a function of the pollutant and precipitation type (i.e., frozen vs. liquid precipitation).

*Chemical Transformation:* CALPUFF includes options for parameterizing chemical transformation effects using the five species scheme ( $\text{SO}_2$ ,  $\text{SO}_4^-$ ,  $\text{NO}_x$ ,  $\text{HNO}_3$ , and  $\text{NO}_3^-$ ) employed in the MESOPUFF II model or a set of user-specified, diurnally-varying transformation rates. The MESOPUFF II scheme is recommended by IWAQM. It produces secondary fine particulate matter (sulfate and nitrate) from emissions of  $\text{SO}_2$  and  $\text{NO}_x$  and thus allows analyses of visibility impacts. Ambient ozone concentrations are used in the parameterized chemical transformation module as a surrogate for OH radicals during daylight hours. Ambient ammonia concentrations are used together with a temperature and relative humidity-dependent equilibrium relationship to partition nitric acid and nitrate on an hour-by-hour and receptor-by-receptor basis.



**Table 3-2. Major Features of the CALPUFF Dispersion Model**

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- **Source types**
  - Point sources (constant or variable emissions)
  - Line sources (constant or variable emissions)
  - Volume sources (constant or variable emissions)
  - Area sources (constant or variable emissions)
- **Non-steady-state emissions and meteorological conditions**
  - Gridded 3-D fields of meteorological variables (winds, temperature)
  - Spatially-variable fields of mixing height, friction velocity, convective velocity scale, Monin-Obukhov length, precipitation rate
  - Vertically and horizontally-varying turbulence and dispersion rates
  - Time-dependent source and emissions data for point, area, and volume sources
  - Temporal or wind-dependent scaling factors for emission rates, for all source types
- **Interface to the Emissions Production Model (EPM)**
  - Time-varying heat flux and emissions from controlled burns and wildfires
- **Efficient sampling functions**
  - Integrated puff formulation
  - Elongated puff (slug) formulation
- **Dispersion coefficient ( $\sigma_y$ ,  $\sigma_z$ ) options**
  - Direct measurements of  $\sigma_y$  and  $\sigma_z$
  - Estimated values of  $\sigma_y$  and  $\sigma_z$  based on similarity theory
    - AERMOD turbulence profiles
    - Original turbulence profiles
  - Pasquill-Gifford (PG) dispersion coefficients (rural areas)
  - McElroy-Pooler (MP) dispersion coefficients (urban areas)
  - CTDM dispersion coefficients (neutral/stable)
- **Vertical wind shear**
  - Puff splitting
  - Differential advection and dispersion
- **Plume rise**
  - Buoyant and momentum rise
  - Stack tip effects
  - Building downwash effects
  - Partial penetration
  - Vertical wind shear
- **Building downwash**
  - Huber-Snyder method
  - Schulman-Scire method
  - PRIME method
- **Complex terrain**
  - Steering effects in CALMET wind field
  - Optional puff height adjustment: ISC3 or "plume path coefficient"
  - Optional enhanced vertical dispersion (neutral/weakly stable flow in CTDMPLUS)

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**Table 3-2. Major Features of the CALPUFF Dispersion Model (Cont'd)**

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- **Subgrid scale complex terrain (CTSG option)**
  - Dividing streamline,  $H_d$ , as in CTDMPLUS:
    - Above  $H_d$ , material flows over the hill and experiences altered diffusion rates
    - Below  $H_d$ , material deflects around the hill, splits, and wraps around the hill
- **Dry Deposition**
  - Gases and particulate matter
  - Three options:
    - Full treatment of space and time variations of deposition with a resistance model
    - User-specified diurnal cycles for each pollutant
    - No dry deposition
- **Overwater and coastal interaction effects**
  - Overwater boundary layer parameters (COARE algorithm or OCD-based method)
  - Abrupt change in meteorological conditions, plume dispersion at coastal boundary
  - Plume fumigation
- **Chemical transformation options**
  - Pseudo-first-order chemical mechanism for  $\text{SO}_2$ ,  $\text{SO}_4^-$ ,  $\text{NO}_x$ ,  $\text{HNO}_3$ , and  $\text{NO}_3^-$  (MESOPUFF II method)
  - Pseudo-first-order chemical mechanism for  $\text{SO}_2$ ,  $\text{SO}_4^-$ ,  $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{HNO}_3$ , and  $\text{NO}_3^-$  (RIVAD/ARM3 method)
  - User-specified diurnal cycles of transformation rates
  - No chemical conversion
- **Wet Removal**
  - Scavenging coefficient approach
  - Removal rate a function of precipitation intensity and precipitation type

### ***3.1.3 Major Features of Postprocessors (CALPOST and POSTUTIL)***

The two main postprocessors of interest for BART applications are the CALPOST and POSTUTIL programs. CALPOST is used to process the CALPUFF outputs, producing tabulations that summarize the results of the simulations, identifying, for example, the highest and second-highest hourly-average concentrations at each receptor. When performing visibility-related modeling, CALPOST uses concentrations from CALPUFF to compute light extinction and related measures of visibility (haze index in deciviews), reporting these for a 24-hour averaging time.

The CALPOST processor contains several options for evaluating visibility impacts, including the method described in the BART guidance, which uses monthly average relative humidity values. CALPOST contains implementations of the IWAQM-recommended and FLAG-recommended visibility techniques and additional options to evaluate the impact of natural weather events (fog, rain and snow) on background visibility and visibility impacts from modeled sources.

The POSTUTIL processor is a program that allows the cumulative impacts of multiple sources from different simulations to be summed, can compute the difference between two sets of

predicted impacts (useful for evaluating the benefits of BART controls), and contains a chemistry module to evaluate the equilibrium relationship between nitric acid and nitrate aerosols. This capability allows the potential non-linear effects of ammonia scavenging by sulfate and nitrate sources to be evaluated in the formation of nitrate from an individual source. CALPUFF makes the full ambient ammonia concentration available to each puff without regard for any scavenging by other puffs. POSTUTIL corrects for such scavenging when the puffs generated by the CALPUFF model overlap, as could be the case for a single source when the wind speed is low, or when nitrate formation is to be attributed to each of several sources that are in a cluster and whose plumes overlap,

POSTUTIL will also compute the impacts of individual sources or groups of sources on sulfur and nitrogen deposition into aquatic, forest and coastal ecosystems. The postprocessor allows the changes in deposition fluxes resulting from changes in emissions to be quantified. For example the output of POSTUTIL and CALPOST can be used as input into an Acid Neutralizing Capacity (ANC) analysis, or for comparison to Deposition Analysis Thresholds (DATs).

## **3.2 Discussion of CALPUFF Applicability and Limitations**

### ***3.2.1 Transport and Diffusion***

According to the IWAQM Phase 2 report (page 18), “CALPUFF is recommended for transport distances of 200 km or less. Use of CALPUFF for characterizing transport beyond 200 to 300 km should be done cautiously with an awareness of the likely problems involved.”<sup>6</sup>

IWAQM’s 200-km limitation derives from the observation that, when compared to the data of the Cross Appalachian Tracer Experiment (CAPTEX), the basic configuration of CALPUFF overestimated inert tracer concentrations by factors of 3 to 4 at receptors that were 300 to 1000 km from the source. The apparent reason was insufficient horizontal dispersion of the simulated plume, presumably because an actual large plume does not remain coherent in the presence of vertical wind shears that typically occur, especially during the night, and of horizontal wind shears over the large puffs that arise over long transport distances.

To better represent such situations, an optional puff splitting algorithm has since been added to CALPUFF to simulate wind shear effects across a well-mixed individual puff by dividing the puff horizontally and vertically into two or more pieces. Differential rates of transport among the new puffs thus generated can increase the horizontal spread of the material in the plume due to vertical wind speed shear and wind direction shear. The horizontal puff splitting algorithm is

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<sup>6</sup> The IWAQM presentation at EPA’s 6<sup>th</sup> Modeling Conference provides the background for this recommendation: “The IWAQM concludes that CALPUFF be recommended as providing unbiased estimates of concentration impacts for transport distances of order 200 km and less, and for transport times of order 12 hours or less. For larger transport times and distances, our experience thus far is that CALPUFF tends to underestimate the horizontal extent of the dispersion and hence tends to overestimate the surface-level concentration maxima. This does not preclude the use of CALPUFF for transport beyond 300 km, but it does suggest that results in such instances be used cautiously and with some understanding.” (From page D-12 of the IWAQM Phase 2 report.)

designed to allow large puffs that may grow to be several grid cells or more in size to split into smaller puffs that can then more accurately respond to variations in the local wind field across the original large puff. This will also tend to increase horizontal dispersion of the plume. Since the creation of additional puffs via puff splitting will increase the computational requirements of the model, possibly substantially, puff splitting is not enabled by default, but can be turned on at the option of the user. Puff splitting may be appropriate for transport distances over 200 to 300 km, or possibly over shorter distances in complex terrain.

Turning to the shorter distance end of the transport range, the CALPUFF section of Appendix A of the *Guideline on Air Quality Models* (40 CFR 51, Appendix W) states, "CALPUFF is intended for use on scales from tens of meters from a source to hundreds of kilometers." This is supported by the IWAQM Phase 2 report, which indicates that the diffusion algorithms in CALPUFF were designed to be suitable for both short and long distances. In this regard, CALPUFF does contain algorithms for such near-field effects as plume rise, building downwash, and terrain impingement and includes routines that deal with the computational difficulties encountered when applying a puff model in the field near to a source.

The recommendations for regulatory use in Appendix A of the *Guideline on Air Quality Models* state, "CALPUFF is appropriate for long range transport (source-receptor distance of 50 to several hundred kilometers)", but provisions for using CALPUFF in the near-field in "complex flow" situations are also included in the regulatory guidance. Complex flow situations may include complex terrain, coastal areas, situations where plume fumigation is likely, and areas where stagnation, flow reversals, recirculation or spatial variability in wind fields (e.g., as due to changes in valley orientation) are important.

The tracer studies with which CALPUFF transport and diffusion capabilities were evaluated in the IWAQM Phase 2 report were generally over distances greater than 50 km. More recently, additional studies of model performance have been performed at shorter distances, including at a power plant in New York state in complex terrain (at source-receptor distances of 2 to 8.5 km) and a second power plant in Illinois in simple terrain (at source-receptor distances in arcs ranging from 0.5 km to 50 km from the stack) (Strimaitis et al., 1998). Other CALPUFF evaluation studies over short-distances include ones by Chang et al. (2001) and Morrison et al. (2003). These studies demonstrate good model performance over source-receptor distances from a few hundred meters to 50 km.

An important factor in the performance of CALPUFF is the choice of dispersion coefficients. The EPA has defined the "regulatory default" option in CALPUFF to allow either Pasquill-Gifford (PG) or turbulence-based dispersion coefficients. CALPUFF has been evaluated and shown to perform better using turbulence-based dispersion for tall stacks (Strimaitis et al., 1998). CALPUFF with turbulence-based dispersion has also been evaluated for overwater transport and coastal situations (Scire et al., 2005). In many other studies, including AERMOD evaluation studies conducted by EPA, the use of PG-dispersion, or more specifically the lack of a convective probability density function (pdf) module, has been demonstrated to result in underprediction of peak concentrations.

In November 2005, EPA approved the AERMOD model, which relies on turbulence-based dispersion, as a regulatory Guideline Model<sup>7</sup>. The ISCST3 model and its PG dispersion coefficients are being phased out as an acceptable regulatory approach. However, EPA Region IV has indicated that the application of turbulence-based dispersion coefficients in CALPUFF needs to be further demonstrated before they are approved for BART application. They will consider accepting the use of turbulence dispersion coefficients on a case-by-case basis for sources that are close to Class I areas.

For regional haze light extinction calculations, use of a plume-simulating model such as CALPUFF is appropriate only when the plume is sufficiently diffuse that it is not visually discernible as a plume *per se*, but nevertheless its presence could alter the visibility through the background haze. The IWAQM Phase 2 report states that such conditions occur starting 30 to 50 km from a source. In this light, the BART guidance strongly recommends using CALPUFF for source-receptor distances greater than 50 km but also presents CALPUFF as an option that can be considered for shorter transport distances.

As discussed above, there do not appear to be any scientific reasons why CALPUFF cannot be used for even shorter transport distances than 30 km, though, as long as the scale of the plume is larger than the scale of the output grid so that the maximum concentrations and the width of the plume are adequately represented and so that the sub-grid details of plume structure can be ignored when estimating effects on light extinction. The standard 1-km output grid that has been established for Class I area analyses should serve down to source-receptor distances somewhat under 30 km; how much closer than 30 km will depend on the topography and meteorology of the area and should be evaluated on a case-by-case basis. For extremely short transport distances, depiction of the concentration distribution will require a grid that is finer than 1 km. (For reference, the width of a Gaussian plume,  $2\sigma_y$ , is roughly 1 km after 10 km of travel distance, assuming Pasquill-Gifford dispersion rates under neutral conditions.)

As an additional consideration, if the plume width is small compared to the visual range, the atmospheric extinction along a typical sight path of tens of kilometers through the plume will be inhomogeneous and the simple CALPOST point estimate of regional light extinction at a receptor point will not be correct. However, the effect of averaging light extinction estimates for 24 hours, during which the plume location shifts over various receptor points, is likely to mitigate this problem to some degree and suggests that using CALPUFF at distances under 30 km will often be appropriate. For the narrow plumes that result from short transport distances, though, the modeled peak 24-hr average extinction at a receptor will tend to overstate the effect of the source on regional haze.

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<sup>7</sup> *Revision to the Guideline on Air Quality Models: Adoption of a Preferred General Purpose (Flat and Complex Terrain) Dispersion Model and Other Revisions; Final Rule.* 70 FR 68218-68261, 9 November 2005.

The U.S. EPA has suggested that the plume visibility model, PLUVUE-II, could be used in lieu of CALPUFF for simulating visibility effects at such short distances.<sup>8</sup> PLUVUE-II is a Gaussian model that simulates the dispersion, chemical conversion, and optical effects of emissions of particles, SO<sub>2</sub>, and NO<sub>x</sub> from a single source. Its outputs include the discoloration of the sky by the plume (so called “plume blight”) and the effect of the plume on visibility along user-selected sight paths that pass through the plume. The impacts of the plume on visibility depend not only on the plume composition, but also on the sight path chosen and its direction relative to the axis of the plume and the location of the sun. It isn’t clear how such sight-path dependent results could be compared to the 0.5 and 1.0 deciview thresholds in the BART guidance. Since CALPUFF is designed to be useful for short transport distances (with features such as the simulation of plume downwash caused by structures at the source), CALPUFF seems more appropriate than PLUVUE-II for evaluating source impact at short distances for BART assessment purposes.

### 3.2.2 Aerosol Constituents

#### *Primary PM<sub>2.5</sub>*

Appendix A of the *Guideline on Air Quality Models* (40 CFR 51, Appendix W) states that CALPUFF can treat primary pollutants such as PM<sub>10</sub>. In actuality, CALPUFF can simulate PM<sub>10</sub> or PM<sub>2.5</sub> or some other size range, because the assumed size distribution of the particles is a user input. The smaller the particles, the more they disperse like an inert gas. In most cases, the dispersion of inert PM<sub>2.5</sub> particles will be only minutely different from that of an inert gas, but the behavior of larger particles will differ.

A particularly important contributor to PM concentrations is the rate of deposition to the surface. PM<sub>2.5</sub> particles, which have a mass median diameter around 0.5 µm, have an average net deposition velocity of about 1 cm/min (or about 14 m/day) and thus the deposition of fine particles is usually not significant except for ground-level emissions. On the other hand, coarse particles (those PM<sub>10</sub> particles larger than PM<sub>2.5</sub>) have an average deposition velocity of more than 1 m/min (or 1440 m/day), which is significant, even for emissions from elevated stacks.

CALPUFF includes parametric representations of particle and gas deposition in terms of atmospheric, deposition layer, and vegetation layer “resistances” and, for particles, the gravitational settling speed. Gravitational settling, which is of particular importance for the coarse fraction of PM<sub>10</sub>, is accounted for in the calculation of the deposition velocity. Effects of inertial impaction (important for the upper part of the PM<sub>10</sub> distribution) and Brownian motion (important for small, sub-micron particles) and wet scavenging are also addressed. The BART guidance recommends that fine particulate matter (less than 2.5 µm diameter), which has higher light extinction efficiency than coarse particulate matter (2.5-10 µm diameters), should be treated separately in the model. CALPUFF allows for user-specified size categories to be treated as

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<sup>8</sup> However, for the reasons given in this paragraph, VISTAS does not recommend PLUVUE-II for BART application

separate species, which includes calculating size-specific dry deposition velocities for each size category.

A primary  $PM_{2.5}$  emission from coal-fired electric generating units (EGUs) that is of relevance to visibility calculations is that of primary sulfate. Although primary sulfate emissions account for only a small fraction of the total sulfur emissions from such sources, it may be important to simulate their effect with CALPUFF, especially at shorter distances before significant formation of secondary sulfate conversion from  $SO_2$  has taken place.

### ***Sulfur Dioxide and Secondary Particulate Sulfate***

The MESOPUFF-II chemistry algorithm used in CALPUFF<sup>9</sup> simulates the gas phase oxidation of sulfur dioxide to sulfate by a linear transformation rate that was developed using regression relationships derived from the analysis of chemical conversion rates produced by a complex photochemical box model (see Scire et al., 1984, for a description of the development of the chemical module). As in all empirically-derived models, the relationships are based on easily-computed or observed parameters that are used as surrogates for the factors that control  $SO_2$  oxidation.

The surrogate factors included in the parameterized chemistry during the daytime hours include solar radiation intensity, ambient ozone concentration, and atmospheric stability class. For example, gas phase  $SO_2$  oxidation is a function of OH radical concentrations. Ozone concentrations are correlated with OH radical concentrations during daytime hours, and their use in the daytime  $SO_2$  conversion rate in CALPUFF is based on this correlation relationship. The philosophy is that OH radical measurements are not available and cannot easily be computed within a model like CALPUFF, but ozone is commonly measured throughout the country, so the use of the well-known surrogate variable (ozone) is more useful in the empirical relationship than factors that are unknown or have a high degree of uncertainty. The same logic applies to the other variables in the relationship. They are surrogates for factors that the regression analysis has shown to be important in  $SO_2$  oxidation rates. At night, the  $SO_2$  conversion is set to a constant low value (default is 0.2%/hr). Aqueous phase oxidation of  $SO_2$  is represented by an additive term that varies with relative humidity and peaks at 3%/hr at 100% relative humidity. CALPUFF represents the chemical conversion as a linear process because it requires linear independence between puffs, although as explained below, non-linear behavior in nitrate formation can be modeled.

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<sup>9</sup> CALPUFF offers two options for parameterizing chemical transformations: the 5 species ( $SO_2$ ,  $SO_4^{2-}$ ,  $NO_x$ ,  $HNO_3$ , and  $NO_3^-$ ) MESOPUFF-II system and the 6 species RIVAD system (which treats NO and  $NO_2$  separately).

IWAQM recommends using the MESOPUFF-II system with CALPUFF. The RIVAD system is believed to be more appropriate for clean environments, however, and therefore was used in the Southwest Wyoming Regional CALPUFF Air Quality Modeling Study in 2001. For the VISTAS region, the IWAQM- and FLM-recommended MESOPUFF-II chemistry is most appropriate.

The IWAQM Phase 2 report concludes that this chemistry algorithm is adequate for representing the gas phase sulfate formation but that it does not adequately account for the aqueous phase oxidation of SO<sub>2</sub>. Actual aqueous phase oxidation in clouds or fog can proceed at rates much greater than 3% per hour, leading IWAQM to suggest that sulfate might be underestimated in such situations. However, aqueous phase oxidation depends on liquid water content, not relative humidity. In reality, liquid water does not exist in the atmosphere at relative humidity much below 100%, while the CALPUFF aqueous reaction term produces sulfate at lower relative humidity. This can lead CALPUFF to overestimate sulfate concentrations when the humidity is high but the cloud water that enables aqueous conversion is not present. Therefore, the direction of the bias in the aqueous chemistry simulation of sulfate formation can vary.

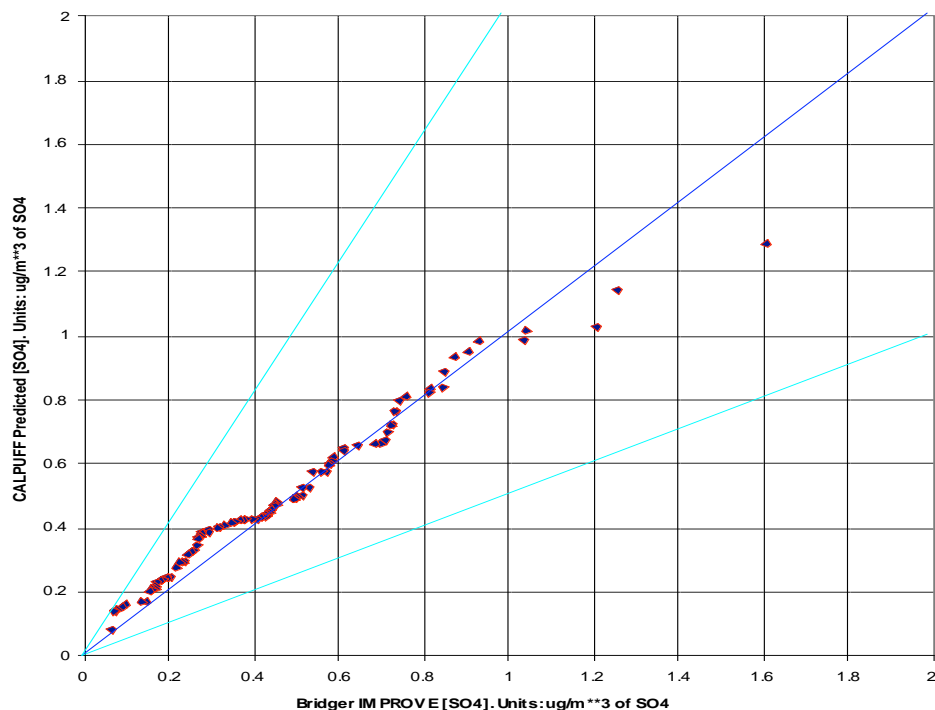
Other potential sources of error in the sulfate formation mechanism of CALPUFF include (1) overestimation of sulfate formation when NO<sub>x</sub> concentrations in the plume are high and in actuality they deplete the local availability of ozone and hydrogen peroxide for oxidizing the SO<sub>2</sub>; and (2) lack of direct consideration of the effect of temperature on the conversion rates, which may cause the model to overstate sulfate formation on cold days (below 10°C or 50°F) (Morris et al., 2003). However, in CALPUFF, the effects of temperature are, to some degree, compensated for indirectly by the use of the solar radiation surrogate variable in the empirical conversion equations.

Whether these potential errors are important will depend on the setting. For example, Figure 3-2 shows a comparison of predicted and observed 24-hour sulfate concentrations, due to a large number of SO<sub>2</sub> sources, at the Pinedale IMPROVE site in Wyoming for the 1995 period (Scire et al., 2001). Overall, in this case there was very little bias in the sulfate predictions. Whether CALPUFF predictions would compare as well with measurements in the Southeast remains to be seen.

CALPUFF does not identify the chemical form of the sulfate compound that results from its reactions, which will generally be some form of ammoniated sulfate whose degree of neutralization will depend on the availability of ammonia in the atmosphere. This consideration, which has been found to be relevant for calculating light extinction in the VISTAS region, is not addressed by CALPUFF or CALPOST.

In most applications, the ozone concentrations required for the sulfate formation calculations are derived from ambient measurements, although concentrations simulated by regional models can be used.





**Figure 3-2. Observed vs. CALPUFF-predicted 24-hour sulfate concentrations at the IMPROVE monitoring site in Pinedale, Wyoming for 1995.**

### *NO<sub>x</sub> and Secondary Ammonium Nitrate*

The MESOPUFF-II chemistry algorithm used in CALPUFF simulates the oxidation of NO<sub>x</sub> to nitric acid and organic nitrates (both gases) by transformation rates that depend on NO<sub>x</sub> concentration, ambient ozone concentration, and atmospheric stability class during the day. The conversion rate at night is set at to a constant value (default is 2.0 %/hr). The temperature- and humidity-dependent equilibrium between nitric acid gas and ammonium nitrate particles is taken into account when estimating the ammonium nitrate particle concentration, an equilibrium that depends on the ambient concentration of ammonia. The user supplies the value of the ambient concentration of ammonia. CALPUFF assumes that the sulfate reacts preferentially with that ammonia to form ammonium sulfate and the left over ammonia is available to form ammonium nitrate.

The IWAQM Phase 2 report considers that this mechanism is adequate for representing nitrate chemistry. Potential situations where this assumption may not be correct, however, include (1) plumes with high concentrations of NO<sub>x</sub> that deplete the ambient ozone and thus limit the

transformation of  $\text{NO}_x$  to nitric acid in the plume; and (2) when ambient temperature is below 10 C, and thus the transformation rate is much slower and the nitrate concentration may be lower than that simulated by CALPUFF (Morris et al., 2003). In both cases, CALPUFF may overestimate the amount of nitrate that is produced. In particular, the impact of ammonium nitrate concentrations on visibility at Class I areas in the VISTAS region is greatest in the winter, when temperatures are lowest, the nitrate concentrations are the greatest, and the sulfate concentrations tend to be the least. CALPUFF may overstate the impacts of  $\text{NO}_x$  emissions at those times, especially in the colder northern states. This potential overestimate of nitrate was not evident, however, in an evaluation of CALPUFF-modeled nitrate against actual observational data in the Wyoming study, as shown in Figure 3-3a (Scire et al., 2001),

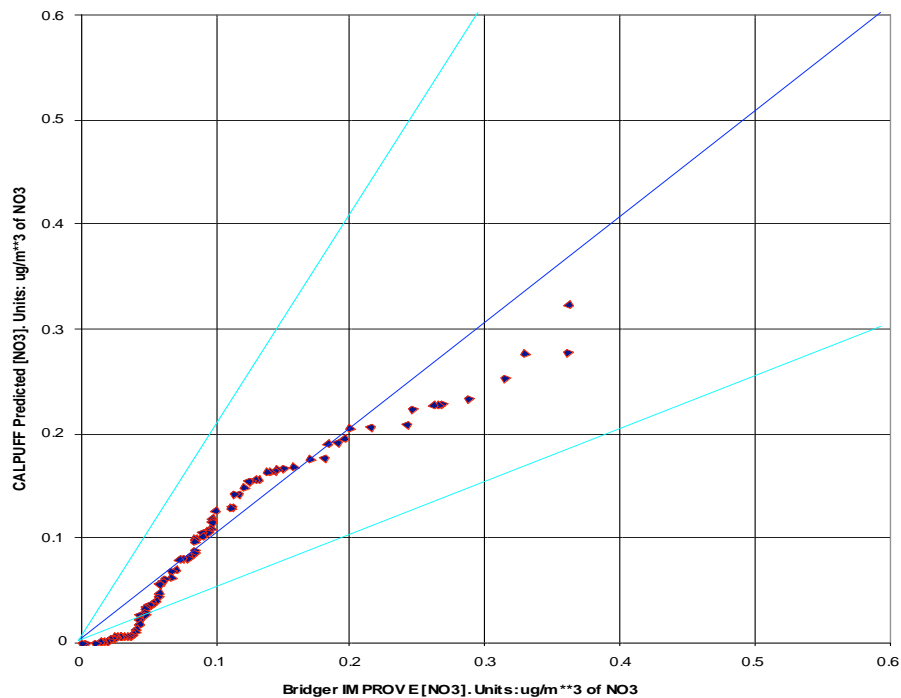
Another factor in the calculation of nitrate is that CALPUFF makes the full amount of the background concentration of ammonia available to each puff, and that amount is scavenged by the sulfate in the puff. If puffs overlap, then that approach could overstate the amount of ammonium nitrate that is formed in total if, in reality, the combined scavenging by the overlapping puffs at a location would deplete the available ammonia enough that the combined nitrate formation was limited by the availability of ammonia. This effect of such ammonia limiting can be large in summer; for a source 75 km west of Mammoth Cave National Park, one modeling analysis found the maximum light extinction impact of the source to be 7.4% (roughly 0.74 deciviews) at the park when CALPUFF was used without consideration of ammonia limiting and about 30% less, between 5.5 and 5.8% (roughly 0.55 to 0.58 dv), when the effect of ammonia limiting was considered (Escoffier-Czaja and Scire, 2002).

To address the issue, since 1999 (i.e., after the IWAQM Phase 2 report) the CALPUFF system has included the optional POSTUTIL postprocessing program, which repartitions the ammonia and nitric acid concentrations estimated by CALPUFF to reflect potential ammonia-limiting effects on the development of nitrate. This allows non-linearity associated with ammonia limiting effects to be included in the CALPUFF model estimates. POSTUTIL computes the total sulfate concentrations from all sources (modeled sources plus inflow boundary conditions) and estimates the amount of ammonia available for total nitrate formation after the preferential scavenging of ammonia by sulfate. That is, as new sulfate, nitrate or ammonia from the source of interest is added to an existing mix of pollutants, POSTUTIL will estimate both the nitrate formed from the new source and the change in background nitrate as a result of the incremental depletion of ammonia (due to the new sulfate and nitrate) or addition of ammonia (from a new source of ammonia).

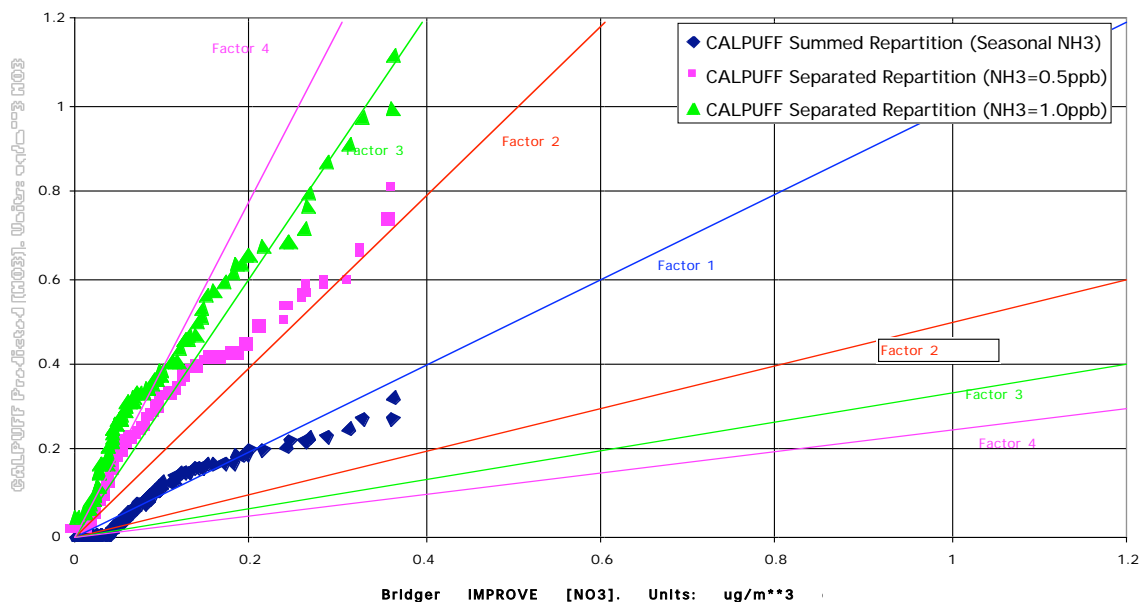
Reliable estimates of the ambient concentrations of ammonia, especially with the temporal and spatial resolution that would be optimal for use with CALPUFF, are needed to take full advantage of the increased accuracy provided by POSTUTIL. The processor requires estimated concentrations of ammonia throughout the modeling domain and period. Such estimates can be inferred from CASTNet measurements, which are integrated over a week, from 24-hr SEARCH measurements, or from the output of a regional photochemical model such as CMAQ or CAMx. The CASTNet network is fairly sparse and the uncertainty in the ammonia measurements is large,

so defining the ammonia concentration throughout the Southeast would require extensive interpolation or extrapolation from the measured values. The quality of the SEARCH measurements is much better, but there are only 8 sites and they do not cover the entire VISTAS domain. Modeled concentrations have the advantage of being resolved in space and time, but their accuracy should be evaluated by comparison with measurements wherever possible.

Benefit is obtained by considering seasonal trends of ammonia and using POSTUTIL to determine the diurnal variability in available ammonia due to the daily cycle of nitrate formation associated with temperature and relative humidity effects. For example, results of the Wyoming study (see Figure 3-3a) show that POSTUTIL adjustments produced daily average nitrate concentrations well within the factor of two lines and with very little mean bias. On the other hand, analysis of the same results with use of constant ammonia of 0.5 ppb or 1.0 ppb produced consistent overpredictions of nitrate by factors of 2-3 and 3-4, respectively, as shown in Figure 3-3b (Scire et al., 2003).



**Figure 3-3a. Observed vs. CALPUFF-predicted 24-hour nitrate concentrations at the IMPROVE monitoring site in Pinedale, Wyoming for 1995 using the ammonia limiting method. (Scire et al., 2001)**



**Figure 3-3b. Observed vs. CALPUFF-predicted 24-hour nitrate concentrations at the IMPROVE monitoring site in Pinedale, Wyoming for 1995 using the ammonia limiting method (blue), constant ammonia at 0.5 ppb (pink) and constant ammonia at 1.0 ppb (green). (Scire et al., 2003)**

### *Secondary Organic Aerosol*

Ongoing research studies at several Class I areas throughout the country (Fallon and Bench, 2004) and at SEARCH sites in the Southeast (Edgerton et al., 2004) are finding that, typically, 90 to 95% of the rural organic carbon fine particle concentration consists of modern carbon (e.g., that from the burning of vegetation and deriving from VOC emissions from vegetation) and only 5 to 10% is attributable to man's burning of fossil fuels. In addition, a field study at Great Smoky Mountains National Park in August 2002 (Tanner, et al., 2005) found that an average of 83% of the fine carbon was modern carbon

According to IMPROVE measurements, organics account for roughly 10% of the particle-caused light extinction in Class I areas in the Southeast. We can thus conclude that, in general, secondary organic carbon particles derived from anthropogenic fossil fuel burning emissions are unlikely to have a large impact (around 1%) on current visibility. (Man-caused burning of vegetation can have significant localized, short-term impacts, however.)

Current organic fine particle concentrations in the Southeast are typically within a factor of 2 of the  $1.4 \mu\text{g}/\text{m}^3$  concentration assumed for natural conditions by the EPA, which means that current fossil fuel burning would contribute less than 2% to visibility in an atmosphere that represents natural conditions. Thus, it is unlikely that VOC and organic particle contributions from BART

sources will cause a large impact to visibility at Class I areas, but a 5% (0.5 dv) localized impact from a particularly large VOC source cannot be dismissed out of hand.

CALPUFF has only rudimentary capabilities for addressing formation of visibility-impairing organic particles from some forms of volatile organic carbon (VOC). The capabilities that do exist include the following.

First, PM<sub>10</sub> emissions (such as from power plants) are often divided into filterable and condensable components, with the condensable mass being 100-200% of the filterable mass. For purposes of visibility analyses with CALPUFF, a fraction of the condensable part is typically treated as organic particles, i.e., it is assumed that a fraction of the condensable components in the PM<sub>10</sub> emissions condense into organic PM<sub>2.5</sub> particles. The size of this organic fraction varies with process and process equipment, and can range from 20 to 100% of the condensable mass. These fine organic particles can be readily modeled by CALPUFF. (The remaining condensable material may be sulfuric, hydrochloric, or hydrofluoric acid.)

Second, a module that treats the formation of secondary organic particles from organic emissions was recently developed and is now part of the CALPUFF system. (Scire et al., 2001). This simplified secondary organic aerosol (SOA) module is a linear, parameterized representation that is currently considered best suited for biogenic organics. It relies on the conventional wisdom that only hydrocarbons with more than six carbon atoms can form significant SOA (Grosjean and Seinfeld, 1989). For example, according to this rule, isoprene (C<sub>5</sub>H<sub>8</sub>) does not make SOA but terpenes do, making pine trees more important biogenic contributors to SOA than oak trees.<sup>10</sup>

Limited evaluation of the performance of CALPUFF at simulating SOA with its biogenic SOA module at one IMPROVE site in a regional modeling study in Wyoming found that 95% of 101 estimated 24-hr SOA concentrations were within 2% of the measured values (Scire et al., 2001). This performance seems promising, although the developers view the SOA module as needing more testing and evaluation.

Thus, CALPUFF includes approaches for dealing with condensable VOC emissions that are characterized as condensable PM<sub>10</sub> and with biogenic VOCs, although the soundness of concentration estimates by these approaches when modeling a plume from a single source is largely untested.<sup>11</sup> The CALPUFF simulation of VOC emissions from sources whose VOC emissions are predominantly anthropogenic is problematic, however. Perhaps the approach used for the simplified biogenic SOA module may be extended to anthropogenic VOCs when speciated VOC emissions information is available. If only those VOCs with more than six carbon atoms are presumed to be of importance, this eliminates many anthropogenic sources of VOC emissions. For example, the fugitive emissions of butane and ethane during petroleum processing

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<sup>10</sup> Recent research suggests that isoprene may be a SOA precursor, however.

<sup>11</sup> Note that neither of these VOC-related simulation approaches is described in the current (Version 5) CALPUFF User's Guide dated January 2001. See the Wyoming report referenced above for a description of this module.

are not important, while aromatic emissions (such as of toluene and xylene) are considered by the SOA module's mechanism. Development, testing, and evaluation would be needed before one could rely on such a module for estimating SOA from anthropogenic SOA emissions, though.

Therefore, to demonstrate the visibility impacts of VOC emissions from BART-eligible sources, means other than CALPUFF will be needed. A technical approach using a regional photochemical model to evaluate visibility impacts of VOC emissions is presented in Section 4.1.3. CALPUFF can be used to estimate the contribution from the primary condensable fraction of PM<sub>10</sub> emissions, though.

### 3.2.3 Regional Haze

Calculation of the impact of the simulated plume particulate matter component concentrations on light extinction is carried out in the CALPOST postprocessor. The formula used is the usual IMPROVE/EPA formula, which is applied to determine a change in light extinction due to changes in component concentrations. Using the notation of CALPOST, the formula is the following:

$$b_{ext} = 3 f(RH) [(NH_4)_2SO_4] + 3 f(RH) [NH_4NO_3] + 4[OC] + 1[Soil] + 0.6[Coarse Mass] + 10[EC] + b_{Ray} \quad (3-1)$$

The concentrations, in square brackets, are in  $\mu\text{g}/\text{m}^3$  and  $b_{ext}$  is in units of  $\text{Mm}^{-1}$ . The Rayleigh scattering term ( $b_{Ray}$ ) has a default value of  $10 \text{ Mm}^{-1}$ , as recommended in EPA guidance for tracking reasonable progress (EPA, 2003a).

There are a few important differences in detail and in notation between the CALPOST formula for estimating light extinction (i.e., Equation 3-1) and that of IMPROVE and EPA. First, the *OC* in the formula above represents organic carbonaceous matter (OMC in IMPROVE's notation), which is 1.4 times the *OC* (i.e., organic carbon alone) in the IMPROVE formula. The *EC* above is synonymous with *LAC* in the IMPROVE formula. CALPOST now offers the option of using the old IMPROVE  $f(RH)$  curve, whose values are documented in the December 2000 FLAG report, or the  $f(RH)$  now used by IMPROVE and EPA (as documented in EPA's regional haze guidance documents). Also, CALPOST sets the maximum *RH* at 98% by default (although the user can change it), while the EPA's guidance now caps it at 95%.

The haze index (HI) is calculated from the extinction coefficient via the following formula:

$$HI = 10 \ln (b_{ext}/10) \quad (3-2)$$

where *HI* is in units of deciviews (dv) and  $b_{ext}$  is in  $\text{Mm}^{-1}$ . The impact of a source is determined by comparing HI for estimated natural background conditions with the impact of the source and without the impact of the source.

## ***CALPOST Methods***

CALPOST uses Equation 3-1 to calculate the extinction increment due to the source of interest and provides various methods for estimating the background extinction against which the increment is compared in terms of percent or deciviews.

For background extinction, the CALPOST processor contains seven techniques for computing the change in light extinction due to a source or group of sources (called Methods 1-7). These are usually reported as 24-hour average values, consistent with EPA and FLM guidance. In addition, there are two techniques for computing the 24-hour average change in extinction (i.e., as the ratio of 24-hour average extinctions, or as the average of 24-hour ratios). A brief summary of the techniques is provided below. Method 2 is the current default, recommended by both IWAQM (EPA, 1998) and FLAG (2000) for refined analyses. Method 6 is recommended by EPA's BART guidance (70 FR 39162).

Methods 4 and 5 use optically measured hourly background extinctions, which represent current actual levels of extinction and thus are not consistent with the "natural conditions" the BART proposal says should be used as a baseline. Methods 1 through 3 and 6 and 7 allow for user inputs of estimated (e.g., natural conditions) background extinction or component concentrations, and thus are consistent with the BART proposal.

Method 1 allows the user to specify a single value of a "dry" background extinction coefficient for each receptor, specify that a certain fraction of that coefficient is due to hygroscopic species, and use relative humidity measurements to vary the extinction hourly via a 1993 IWAQM  $f(RH)$  curve or, optionally, the EPA regional haze  $f(RH)$  curve (EPA, 2003b). The  $RH$  is capped at 98% or a user-selected value (95% for the EPA curve). The same  $f(RH)$  is applied to both the modeled sulfate and nitrate.

For an example of the use of Method 1, one could use the dry particle extinction coefficient of  $9.09 \text{ Mm}^{-1}$  that results from EPA's default natural conditions concentrations, together with an assumption that for natural conditions, say,  $0.9 \text{ Mm}^{-1}$  (or 10%) of this amount results from hygroscopic ammonium sulfate and ammonium nitrate, and then apply  $f(RH)$  to this 10%.

In Method 2, user-specified, speciated monthly concentration values are used to describe the background. When applied to natural conditions, for which EPA's default natural conditions concentrations are annual averages, the same component concentrations would have to be used throughout the year (unless potential refinements to those default values resulted in concentrations that vary during the year). Hourly background extinction is then calculated using these concentrations and hourly, site-specific  $f(RH)$  from a 1993 IWAQM curve (a different one

than that in Method 1) or, optionally, the EPA regional haze  $f(RH)$  curve.<sup>12</sup> Again the  $RH$  is capped at either 98% (default) or a user-selected value (most commonly at 95%).

Method 3 is the same as Method 2, except that any hour in which the  $RH$  exceeds 98% (or the selected maximum) is dropped from the analysis. When 24-hr extinction is computed, no fewer than 6 valid hours are accepted at each receptor; otherwise the value for the day is tabulated as “missing”.

Method 6 is similar to Method 2, except monthly  $f(RH)$  values (e.g., EPA’s monthly climatologically representative values in EPA (2003a, b)) are used in place of hourly values for calculating both the extinction impact of the source emissions and the background conditions extinction. Hourly source impacts, with the effect on extinction due to sulfates and nitrates calculated using the monthly-average relative humidity in  $f(RH)$ , are compared against the monthly default natural background concentrations. Thus the monthly-averaged relative humidity is applied to the hygroscopic components (i.e., sulfate and nitrate) of both the source impact and the background extinction with Method 6.

Method 7 is a new variant of Method 2 that was developed as a result of a ruling by the Assistant Secretary of the Interior for Fish and Wildlife and Parks, in response to a New Source Review case in Montana, that “natural conditions” should reflect the visibility impairment caused by significant meteorological events such as fog, precipitation, or naturally occurring haze (DOI, 2003).<sup>13</sup> Under Method 7, during hours when visibility is obscured by meteorological conditions, the actual measured visibility is used to represent natural conditions instead of the value that is calculated from EPA’s default natural conditions concentrations under Method 2. A recent modification developed in response to FLM comments on Method 7, in which the daily average natural extinction is calculated somewhat differently, is called Method 7’, i.e., “7 prime”.

### ***Refined Estimates of Extinction and Natural Background Visibility***

Separate from the BART discussions, IMPROVE, EPA, and the Regional Planning Organizations are evaluating whether refinements are warranted to the methods recommended in EPA’s guidance to calculate default estimates of natural background visibility. In particular, IMPROVE has recently approved an alternative to the formula (Eq. 3-1) it uses to estimate extinction from particle concentration measurements (Pitchford et al., 2005).

Refinements in the revised IMPROVE formula include the following:

- Adding a sea salt term, including a growth factor due to relative humidity

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<sup>12</sup> Note that the hourly-varying natural background extinction in this method is not consistent with that prescribed by the EPA’s natural conditions guidance (EPA, 2003b), for which a “climatologically-representative”  $f(RH)$  that only varies monthly is to be used. Method 6 uses these monthly average humidity values.

<sup>13</sup> The Secretary’s guidance applies only to Federal Land Managers. EPA’s position on this interpretation of natural conditions is unknown.



- Increasing the factor used to calculate the mass of particulate organic matter (OC in Eq. 3-1) from organic carbon measurements
- Modifying the relative humidity growth formula,  $f(RH)$ , for sulfates and nitrates
- Revising the extinction efficiencies (the numerical constants in Equation 3-1) for sulfates, nitrates, and organic carbon so that they vary with concentration
- Adding a site-specific Rayleigh scattering term to the formula. Values will be calculated by IMPROVE for all Class I areas.

For the purposes of calculating current, future, and natural background visibility at VISTAS Class I areas as part of the reasonable progress analyses, VISTAS intends to present regional air quality modeling results using both the current EPA recommended assumptions and the newly revised aerosol extinction formula. If a BART-eligible source chooses to consider its projected impacts using the newly revised formula as well as the current formula, then modifications would need to be made to CALPOST to carry out calculations with the new algorithm.

## **4. VISTAS' COMMON MODELING PROTOCOL**

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### **4.1 Overview of Common Modeling Approach**

In this section, guidance is provided on the use of the CALPUFF modeling system for two purposes:

- 1) Evaluating whether a BART-eligible source is exempt from BART controls because it is not reasonably expected to cause or contribute to impairment of visibility in Class I areas, and
- 2) Quantifying the visibility benefits of BART control options.

For purpose 1), States must determine whether a source emits any air pollutant (SO<sub>2</sub>, NO<sub>x</sub>, PM, and in certain cases VOC and NH<sub>3</sub>) that “may reasonably be anticipated to cause or contribute to any impairment of visibility” in a Class I area. The States have 3 options to accomplish this:

- A) Conclude that all BART-eligible sources in State are subject to BART.
- B) Demonstrate that all BART-eligible sources in the State together do not cause or contribute to any visibility impairment
- C) Determine if the impact from each individual BART-eligible source is greater than a threshold value.

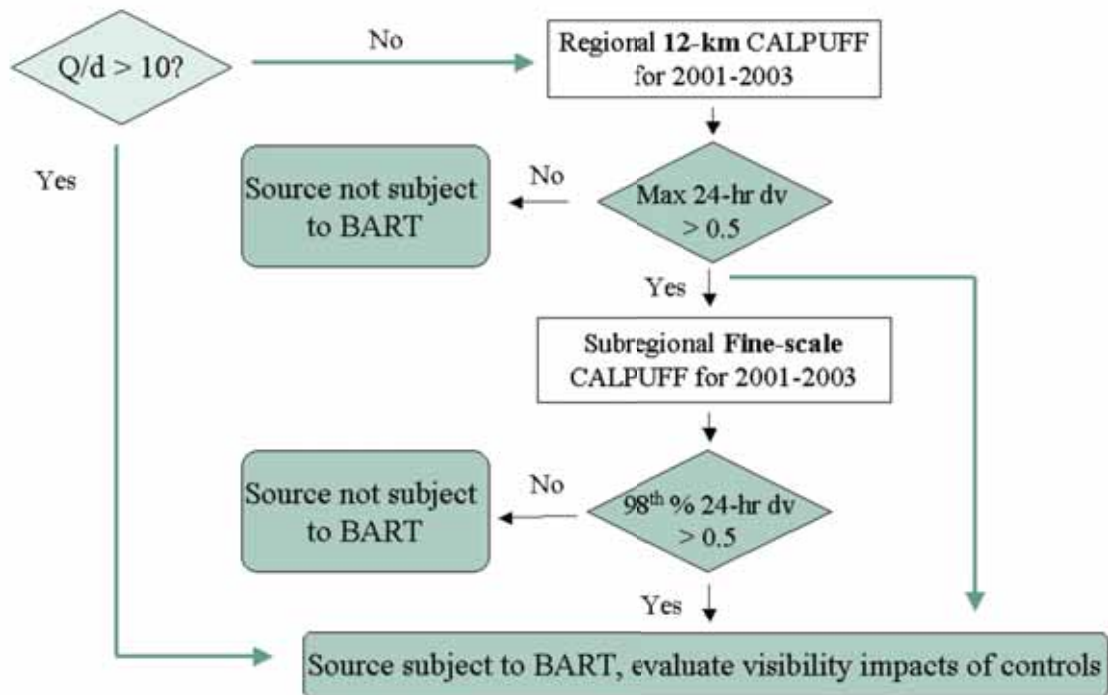
VISTAS States intend to follow Option C (determine if the visibility impact from individual sources exceeds a contribution threshold) for SO<sub>2</sub> and NO<sub>x</sub> emissions. The methods for Option C are described in Section 4.1.1. In early 2006, VISTAS pursued Option B (demonstrate that all BART eligible sources in a State do not impact visibility) for VOC, NH<sub>3</sub> and PM emissions. The approach and results for Option B are described in Section 4.1.3. As a result of this exercise, the VISTAS States have determined that the Option C exemption analyses should also include PM emissions and, for sources with large NH<sub>3</sub> emissions, NH<sub>3</sub>. The States determined that anthropogenic VOC emissions do not cause or contribute to visibility impairment at VISTAS Class I areas and that VOC emissions do not need to be considered in BART analyses.

#### ***4.1.1 BART Exemption Analysis***

As illustrated in Figure 4-1, three steps will evaluate whether a BART-eligible source of SO<sub>2</sub>, NO<sub>x</sub>, or PM is subject to BART:

- 1) VISTAS plans to use Q/d as a presumptive indicator that a source is subject to BART. If Q/d for SO<sub>2</sub> > 10 for 2002 actual emissions, then the State presumes that the source is subject to BART. If the source agrees with this presumption, then no exemption modeling is required and the source can proceed to the BART determination using CALPUFF to evaluate impacts of control options and can perform the engineering analyses. If a source disagrees, the source

may perform fine grid modeling as described in Section 4.4 to determine if its impact is  $< 0.5$  dv.



**Figure 4-1. Flow chart showing the components of the VISTAS common modeling protocol.** Assessment should be made for each Class I Area. (If a source agrees to install the most stringent controls then the modeling steps indicated above and engineering analyses and visibility impact modeling would not be required.)

- 2) An optional initial modeling assessment using the CALPUFF model with the coarse scale 12-km regional VISTAS domain can be used to answer questions whether (a) a particular source may be exempted from further BART analyses and (b) if finer grid CALPUFF analysis were to be undertaken, which Class I areas should be included. Assumptions for the initial modeling assessment are conservative so that a source that contributes to visibility impairment is not exempted in error. If a source is shown not to contribute to visibility impairment using the initial modeling assessment, the source would not be subject to BART and would be exempted from further BART analyses. If a source is shown to contribute to visibility impairment using the initial modeling assessment, the source has the option to undertake finer grid CALPUFF modeling to evaluate further whether it is subject to BART.
- 3) A finer grid CALPUFF modeling analysis using a subregional CALMET domain will be the definitive test as to whether a source is subject to BART.

For large sources that will clearly exceed the initial screening thresholds, this step can be skipped and the analysis may proceed directly to the finer grid modeling analysis, which is described in Section 4.4.

#### ***4.1.2 BART Control Evaluation***

For sources that are determined to be subject to BART controls, part of the BART review process involves evaluating the visibility benefits of different BART control measures. These benefits will be determined by making additional CALPUFF simulations using the same CALMET and CALPUFF configuration as those used in the finer grid analysis of Step 2. The only exception is that the source and emissions data used in the CALPUFF control evaluation simulations will reflect the BART control measures being evaluated. Using the same model configuration will produce an “apples-to-apples” comparison, where differences in impacts are due to the effectiveness of the controls rather than model configuration differences. For example, a control scenario evaluation that uses more conservative assumptions than the base case simulation may produce results showing no or little improvement in visibility impacts. That control scenario run with the same model configuration as the base case may show significant visibility improvement. Therefore, in order to not obscure the response to predicted visibility improvements by differences in the modeling approach, the same model configuration should be used in the BART control evaluation simulation as in the base case simulation.

The base case to which the effectiveness of BART controls is to be compared is the “current emissions” scenario for which the finer grid Step 2 modeling was performed. The postprocessing steps and procedures are the same as in the BART eligibility simulation. Side-by-side comparison of the visibility impacts will be tabulated to quantify the effectiveness of each control scenario relative to the base case.

The modeling evaluation is a unit-by-unit evaluation and can be conducted on a pollutant specific basis. Modeling results are used with the other four statutory factors mentioned in Section 2.1 to decide which control technology, if any, is appropriate. Finally, if a source decides to use the most stringent control technology available, the BART control analysis, including modeling, is not necessary.

#### ***4.1.3 VISTAS’ Treatment of VOC, NH<sub>3</sub>, and PM***

##### ***Volatile Organic Compounds***

CALPUFF is currently not recommended for addressing visibility impacts from VOC because its capability to simulate secondary organic aerosol formation from VOC emissions is not adequately tested, especially for anthropogenic emissions. (Separately, condensable organic carbon can be calculated from PM<sub>10</sub>.)

VISTAS has performed a weight of evidence analysis to demonstrate, using the CMAQ regional air quality model, that the combined VOC emissions from all point sources (BART-eligible and non-BART) in each State do not contribute to visibility impairment. Emissions sensitivity

simulations run for VISTAS by Georgia Institute of Technology using VISTAS' 12 x 12 km grid and CMAQ v 4.3 for episodes in July 2001 and January 2002 demonstrated very low to no response of organic carbon levels and light extinction at Class I areas to changing VOC emissions from all anthropogenic sources in the VISTAS 12-km modeling domain (eastern US). Georgia Tech repeated the sensitivity analyses using the VISTAS 12-km domain and CMAQ v 4.4 with a refined SOA module for summer (Jun 1-Jul 10) and winter (Nov 19-Dec 19) periods in 2002. VOC emissions from all anthropogenic point sources in every VISTAS State were reduced by 100% (i.e., eliminated). The maximum 24-hr impact of all VOC emissions from all point sources throughout the VISTAS domain was thus determined to be less than 0.5 dv (compared to annual average natural background) at every Class I area in the VISTAS domain and in adjacent States. It follows that the impact of any one BART-eligible source would be much less than 0.5 dv. Based on these analyses, the VISTAS States have concluded that VOC emissions from BART sources do not cause or contribute to visibility impairment and do not need to be included in BART analyses.

### ***Ammonia***

EPA has given states the option to address ammonia (NH<sub>3</sub>) emissions from BART-eligible sources. VISTAS also contracted with Georgia Tech to calculate NH<sub>3</sub> emissions sensitivities using CMAQ v 4.4 with a refined SOA module and the same Jun-Jul and Nov-Dec periods in 2002 that were used for the VOC sensitivity evaluation. The NH<sub>3</sub> emissions from all point sources (BART-eligible and not-BART) in every State were reduced by 100% for these analyses. This sensitivity evaluation showed that the collective impact of all VISTAS region point NH<sub>3</sub> emissions is greater than 0.5 dv (compared to annual average natural background) at several Class I areas. When the NH<sub>3</sub> emissions were scaled to represent 100% reduction from only the BART-eligible sources in each State, then the maximum impact of those sources was under 0.5 dv at most, but not all Class I areas. The high values appear to result primarily from emissions from 13 large NH<sub>3</sub> sources. In the absence of those 13 facilities, the scaled NH<sub>3</sub> emissions peak impacts at Class I areas were 0.3 dv or less. Based on these analyses, the VISTAS States recommended that, except for these 13 facilities, NH<sub>3</sub> emissions not be included in BART modeling. States will provide instructions to those 13 sources as to how to evaluate contributions of their NH<sub>3</sub> emissions to visibility impairment. For documentation purposes, in summer 2006 VISTAS is repeating the NH<sub>3</sub> emissions sensitivity calculations, using CMAQ v4.5 with Base F emissions and reducing 100% of NH<sub>3</sub> emissions from only the BART-eligible sources in the VISTAS states.

### ***Primary Particulate Matter***

Primary particulate matter is considered a visibility impairing pollutant. However, the extent to which primary PM from BART-eligible sources contributes to impairment at Class I areas in the southeastern US is not clear. For EGUs, the EPA has determined that emissions reductions of SO<sub>2</sub> and NO<sub>x</sub> under the CAIR rule meet the BART requirements, but these EGUs may still be subject to BART for primary PM. To determine the potential impacts of PM from EGU and non-EGU sources in the VISTAS states, two CMAQ sensitivity runs for the first and third quarters of 2002 were carried out by VISTAS' CMAQ modeling team of ENVIRON, UCR, and Alpine

Geophysics In one run, all primary PM from EGUs was removed while in the other run all primary PM from non-EGU sources was removed. All other CMAQ modeling components were held constant. At almost all Class I areas in the VISTAS region, primary PM emissions contribute to regional haze, with the collective impact of all EGU and non-EGU point primary PM emissions being greater than 0.5 dv compared to annual average natural background. In fact, the impacts of EGU PM emissions alone or of non-EGU PM emissions alone were each mostly greater than 0.5 dv. Although the impacts of BART sources alone would be smaller, the VISTAS States have concluded that all BART-eligible sources need to consider the impacts of their PM emissions.

## **4.2 Optional Source-Specific Modeling**

In some circumstances, a source may want to apply techniques designed to evaluate the impacts in a more detailed way than the standard VISTAS common protocol. A source may propose source-specific modeling procedures to address special issues to the State for State review. For example, sources very close to Class I areas may be better treated by a finer grid resolution than the generic Step 2 “fine” grid resolution meteorological fields provided by VISTAS. In some situations, higher resolution MM5 or other prognostic meteorological datasets may be available than the standard 12-km or 36-km MM5 datasets provided by VISTAS. Because it is not possible to anticipate all of the situations where there would be a benefit to conducting more detailed source-specific analyses, the option to pursue this option is left as an open issue, to be resolved and justified based on specific factors relevant for the source in question.

A source-specific modeling protocol is required for each source. This document should describe the data sources and model configuration, and provide rationale for any changes in the model approach from the common protocol. This source-specific protocol must be provided for review and approval by the State. The State will share the protocol with EPA and the Federal Land Managers for their review. Discussion of approaches to source-specific modeling and an outline of the typical contents of the source-specific protocol are presented in Chapter 5. Discussions with the regulatory authorities should be conducted prior to development of a source-specific protocol to ensure all of the relevant issues are included in the protocol.

## **4.3 Initial Procedure for BART Exemption**

### ***4.3.1 Overview of Initial Approach***

The first step in the common protocol, the initial assessment in Figure 4-1, is a simple procedure to evaluate whether a source can be exempted from BART controls using a consistent set of meteorological and dispersion options. A pre-computed set of meteorological files and a pre-defined CALPUFF input option configuration, based on guidance in the final BART rule (70 FR 39104-39172) and other EPA and FLAG model guidance, will allow relatively simple initial simulations. The regional initial domain is designed to allow any Class I areas within the VISTAS area to be evaluated with a single meteorological database and consistent CALPUFF modeling options. The second important question that this first screening step will answer is, if

initial modeling indicates a source may impact visibility significantly, what Class I areas should be included in a finer grid analysis? Due to the multitude of factors affecting the contribution of a source to visibility in a Class I area, simple screens or rules of thumb alone (such as that the closest Class I area will produce the controlling visibility impacts) are not likely to be universally reliable.

#### ***4.3.2 Discussion of 12-km Initial Exemption Modeling***

##### ***Meteorological Fields***

A regional initial domain and a set of pre-computed regional CALMET meteorological files will be prepared for VISTAS, to allow any Class I areas within the VISTAS area to be evaluated with a consistent meteorological database and consistent CALPUFF modeling options.

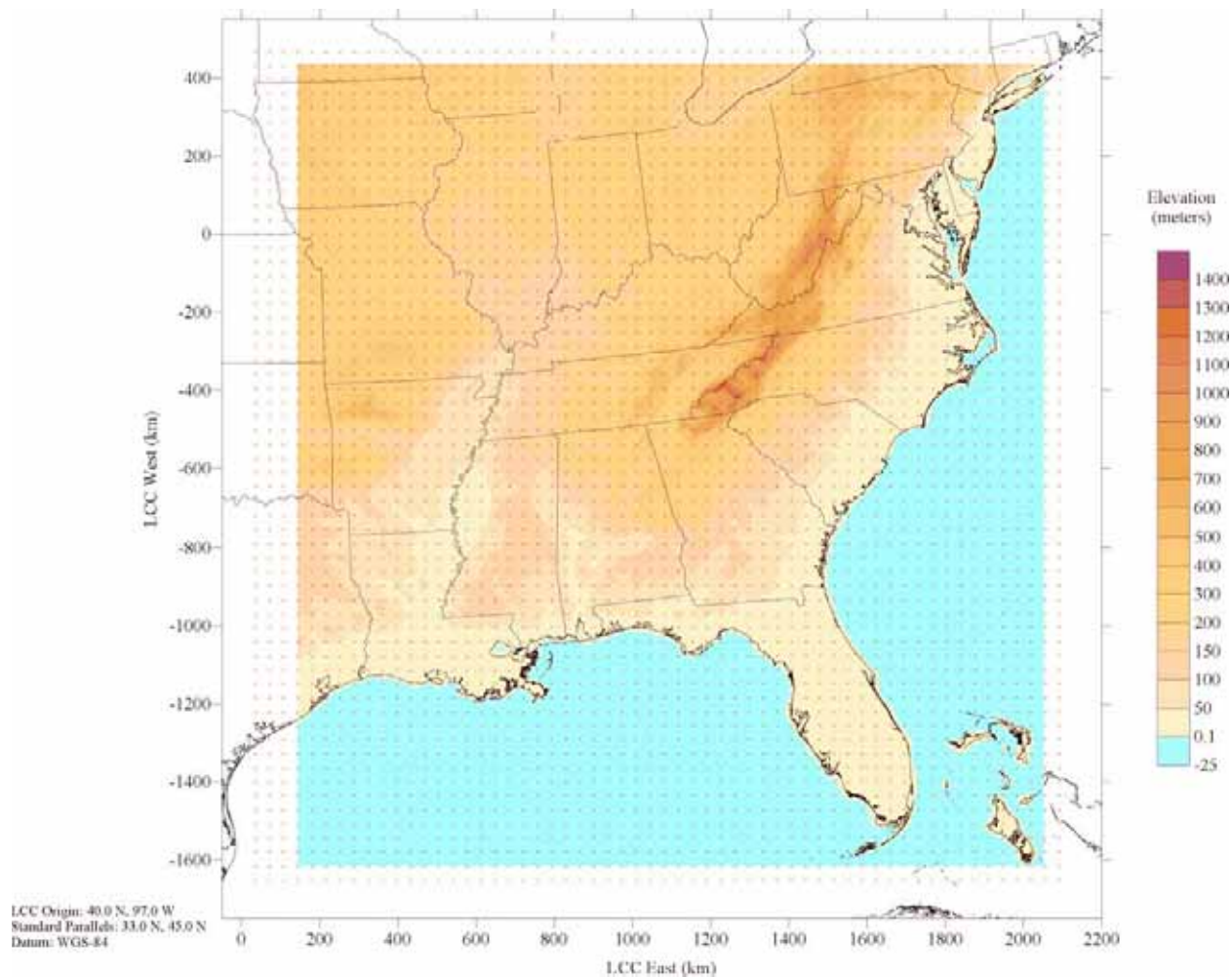
The following three years of MM5 meteorological data have been assembled by VISTAS for use in the regional CALPUFF modeling effort:

- 2001 MM5 dataset at 12 km and 36 km grid (developed for EPA)
- 2002 MM5 dataset at 12 km and 36 km grid (developed by VISTAS)
- 2003 MM5 dataset at 36 km grid (developed by the Midwest Regional Planning Organization).

These data sets have been provided to Earth Tech by VISTAS, and from them Earth Tech has produced annual CALMET meteorological files at 12-km grid resolution for the domain shown in Figure 4-2. The CALMET modeling output files in the form of CALPUFF-ready three-dimensional meteorological files will be available on external hard drives to the States and other parties.

The initial procedure to determine if a BART-eligible source is subject to BART uses the pre-computed CALMET meteorological fields for the years 2001-2003 on the 12-km CALMET domain in Figure 4-2 and simulates with CALPUFF any BART-eligible source to be screened. The CALMET simulations will be developed using the highest resolution MM5 data available for each year (i.e., 36-km MM5 data for 2003, 12-km MM5 data for 2001 and 2002).

The development of the regional CALMET meteorological fields from MM5 data will be conducted in No-Observations (“No-Obs”) mode. The MM5 data already reflect assimilation of observational data and are likely to adequately characterize regional wind patterns that are consistent with the 12-km grid scale. Blending of MM5 data with local observations (which are mainly at the surface) could lead to wind structures that may not be realistic under some conditions and may result in poorer characterization of the regional winds. Thus, the effort required to prepare observational data sets for CALMET for the large regional domain involves considerable effort that may not provide corresponding improvement of the wind field.



**Figure 4-2. VISTAS Regional 12-km Resolution CALMET Modeling Domain (color area with terrain contours). The locations of the 36-km resolution MM5 grid points are shown on the plot.**

For 2003, the 36-km MM5 data will be used as CALMET's initial guess field and then the CALMET diagnostic terrain adjustments (see Section 3.1.1) will be applied to reflect terrain on the scale of the CALMET grid (i.e., 12-km). When the 12-km MM5 (2001 and 2002) data are used, the diagnostic CALMET terrain adjustments will be turned off since the grid resolution of the MM5 data is the same as the CALMET grid and the terrain adjustments on the 12-km grid scale will already be reflected in the MM5 dataset. In this case, the MM5 winds will be interpolated by CALMET to the CALMET layers and CALMET's boundary layer modules will compute mixing heights, turbulence parameters and other meteorological parameters that are required by CALPUFF.



### ***Impact Threshold***

The final BART guidance recommends that the threshold value to define whether a source “contributes” to visibility impairment is 0.5 dv change from natural conditions<sup>14</sup> (although States may set a lower threshold). The 98<sup>th</sup> percentile (8<sup>th</sup> highest annual) 24-hr average predicted impact at the Class I area, as calculated using CALPOST Method 6 (monthly average relative humidity values), is to be compared to this contribution threshold value. For this comparison, the predicted impact at the Class I area on any day is taken to be the highest 24-hr average impact at any receptor in the Class I area on that day. (Note that the receptor where the highest impact occurs can change from day to day.) According to clarification of the BART guidance received from EPA, for a three-year simulation the modeling values to be compared with the threshold are the greatest of the three annual 8<sup>th</sup> highest values or the 22<sup>nd</sup> highest value over all three years combined, whichever is greater.

For the purposes of the initial analysis, however, the *highest value* over the three-year period (not the 98<sup>th</sup> percentile value) is to be compared to the contribution threshold. This ensures a significant measure of conservatism in the initial approach. VISTAS will evaluate the initial CALPUFF results to determine if using the single highest value provides too conservative a screen for exemption purposes. If so, VISTAS may increase the number of exceedances of the contribution threshold that would be allowed and still qualify to exempt a source.

#### ***4.3.3 Model Configuration and Settings for Initial Analysis***

VISTAS will use CALPUFF Version 5.754 and CALMET Version 5.7. These versions contain enhancements funded by the Minerals Management Service (MMS) and VISTAS. They were developed by Earth Tech, Inc. and they are maintained on the CALPUFF website ([www.src.com](http://www.src.com)) for public access. This version includes CALMET, CALPUFF, CALPOST, CALSUM, and POSTUTIL as well as CALVIEW.

The initial analysis uses a CALPUFF computational domain that includes all Class I areas within 300 km of a source. These Class I areas are specified in the CALPUFF control file for analysis. States could decide to require a different value for the maximum distance threshold for the CALPUFF domain, depending on the locations of the Class I areas in their states and other factors such as meteorological conditions and the magnitudes of the emissions from BART-eligible sources. The regional CALMET domain will be unchanged by these adjustments.

Also, the initial approach is designed to significantly reduce the CALPUFF simulation time by restricting the CALPUFF computational domain size to include only areas where significant impacts are feasible rather than the entire regional domain. CALPUFF allows its computational domain to be specified as a subset of the CALMET meteorological domain by settings within the

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<sup>14</sup> As described in Footnote 5 on page 6, States have the option of defining natural conditions as either the annual average default conditions or the average of the 20% best natural condition days.

CALPUFF input file. The advantage of selecting a smaller CALPUFF computational domain in the regional CALPUFF simulations is that CALPUFF run time is proportional to the number and residence time of the puffs on the domain (and other factors such as the number of receptors and the internal time step computed by the model). A CALPUFF domain covering an area 300 km from a source in all directions would involve only 50 x 50 12-km grid cells, which will require modest computational resources.

CALMET output files for the VISTAS regional domain shown in Figure 4-2 will be provided to VISTAS by Earth Tech. These files will be in CALPUFF-ready format, and as such, no CALMET user inputs will be required. An option in CALMET allows finer grid CALMET input files to be calculated from the 12-km CALMET files.

The basic characteristics of the CALMET, CALPUFF and CALPOST configurations for the initial analyses are listed below.

#### ***CALMET Modeling Configuration (12-km initial exemption modeling)***

The CALMET model configuration for the regional CALMET simulations will be defined by Earth Tech in collaboration with the VISTAS States. The basic model configuration will follow the recommended IWAQM guidance (EPA, 1998; Pages A-1 through A-6), except as noted below.

The basic features of the modeling simulation are the following:

- Modeling period: 3 years (2001-2003)
- Meteorological inputs: MM5 data provide initial guess fields in CALMET
- CALMET grid resolution: 12-km (same Lambert Conformal coordinate system and grid cells as the 12-km 2001/2002 MM5 simulations)
- CALMET vertical layers: 10 layers. Cell face heights (meters): 0, 20, 40, 80, 160, 320, 640, 1200, 2000, 3000, 4000.
- CALMET mode: No-Observations mode including option to read overwater data directly from MM5.
- Diagnostic options: IWAQM default values, except as follows: diagnostic terrain blocking and slope flow algorithms used for 2003 simulations (using 36-km MM5 data), but no diagnostic terrain adjustments in 2001 and 2002 simulation (using 12-km MM5 data)
- CALMET options dealing with radius of influence parameters (R1, R2, RMAX1, RMAX2, RMAX3), BIAS, ICALM parameters are not used in No-Observations mode.

- TERRAD (terrain scale) is required for runs with diagnostic terrain adjustments (i.e., the 2003 simulations). Values of ~10-20 km will be tested, and an appropriate value determined.
- Land use defining water: JWAT1 = 55, JWAT2 = 55 (large bodies of water). This feature allows the temperature field over large bodies of water such as the Atlantic Ocean and the Great lakes to be properly characterized by buoy observations.
- Mixing height averaging parameter (MNMDAV) will be determined by Earth Tech for the regional simulations based on sensitivity tests. The purpose of the testing is to optimize the variable to allow spatial variability in the mixing height field, but without excessive noise.
- Geophysical data for regional runs: SRTM-GTOPO30 30-arcsec terrain data, Composite Theme Grid (CTG) USGS 200m land use dataset. References for these and other CALMET datasets can be found on the CALPUFF data page of the official CALPUFF site ([www.src.com](http://www.src.com)).

### ***CALPUFF Modeling Configuration (Initial exemption modeling)***

The CALPUFF model configuration for the regional CALPUFF initial simulations will follow the recommended IWAQM guidance (EPA, 1998; Pages B-1 through B-8), except as noted below:

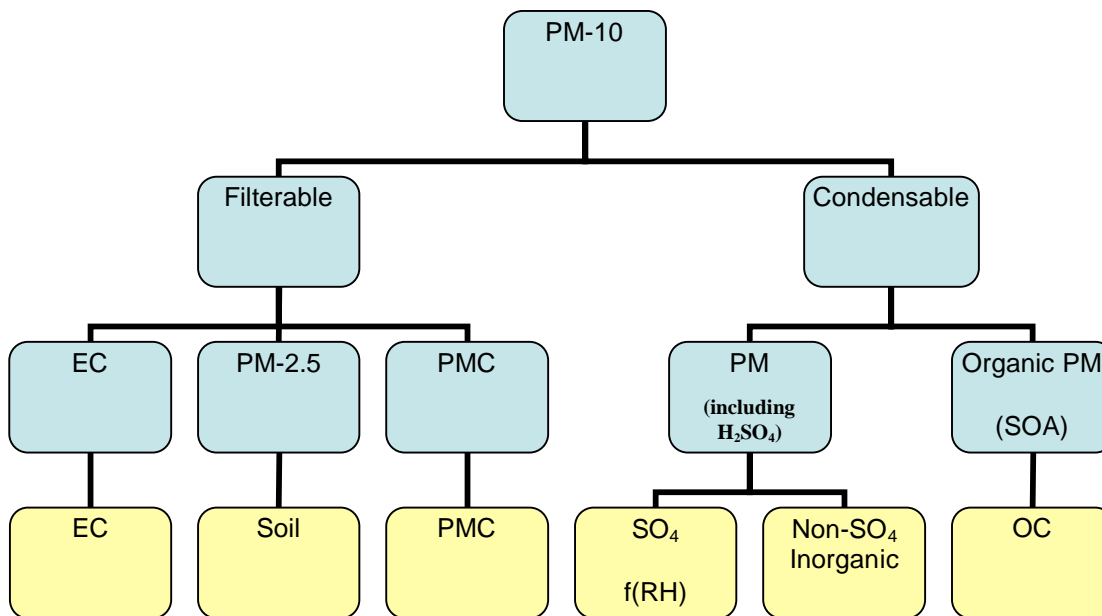
- CALPUFF domain configured to include the source and all Class I areas within 300km of the source plus 50km buffer zone in each direction. CALPUFF is recommended for all source-receptor distances to be considered in the BART analyses.
- Chemical mechanism: MESOPUFF II module
- Species modeled: SO<sub>2</sub>, SO<sub>4</sub>, NO<sub>x</sub>, HNO<sub>3</sub>, NO<sub>3</sub> and particulate matter in size categories of <0.625 μm, 0.625-1.0 μm, 1.0-1.25 μm, 1.25-2.5 μm, 2.5-6.0 μm and 6-10 μm aerodynamic diameters. As noted below, the particulate matter emissions by size category will be combined into the appropriate species for the visibility analysis (i.e., elemental carbon (EC), fine PM or “soil” (< 2.5 μm in diameter), coarse PM (between 2.5-10 μm in diameter) and organics (called secondary organic aerosols (SOA) in the CALPOST postprocessor).
- Emission rates for modeling based on EPA BART guidance, i.e., maximum 24-hour actual emission rate with normal operations from the highest emitting day of the meteorological period modeled (excluding days where start-up, shutdown or malfunctions occurred sometime during the day.) Note that potential emissions are used to determine if a source is BART-eligible, but 24-hour average maximum emissions are used for modeling purposes (70 FR 39162). Pollutants considered include SO<sub>2</sub>, H<sub>2</sub>SO<sub>4</sub>, NO<sub>x</sub> and PM<sub>10</sub>.

Condensable emissions are considered as primary fine particulate matter and allocated equally to the two submicrometer-particle size classes. If actual source emissions data are not available, the modeling should be based on permit limits. If source-specific size

categories are not available, then AP-42 factors may be used for sources where AP-42 factors are available. For sources where AP-42 factors are not available, alternative approaches to speciation are given below.

Excluded from the modeling are pollutants with plant-wide emissions less than *de minimis* levels (40 tons per year for SO<sub>2</sub> and NO<sub>x</sub> and 15 tons per year for PM<sub>10</sub>). *De minimis* levels are plant wide for each visibility-impairing pollutant, so individual units may be modeled even if they have emissions below *de minimis* if the plant total is greater than *de minimis*.

- Particulate emissions speciation: Break down, as appropriate, filterable and condensable particulate matter into the following species categories: elemental carbon (soot), “soil” (fine PM < 2.5 µm diameter), coarse particulate matter (2.5-10 µm diameter) and organics. The process is illustrated in Figure 4-3. If source-specific speciated emissions factors are not available, AP-42 factors or speciation information developed by the National Park Service (<http://www2.nature.nps.gov/air/permits/ect/index.cfm>) can be used to estimate the PM speciation for many source sectors.



**Figure 4-3. Speciation of PM-10 Emissions. (PMC is coarse particulate matter -- 2.5 to 10 µm diameter.)**

Otherwise, assumptions will need to be proposed by the source, and reviewed and approved by the State. Possible acceptable alternative approaches to estimating speciation include the following:

- Speciation profiles developed by the SMOKE emissions model for use in VISTAS' CMAQ regional air quality modeling (available at <http://www.vistas-sesarm.org/BART/calpuff.asp>).
  - The approach described in a memo available at <http://www.vistas-sesarm.org/BART/calpuff.asp>, which provides reasonably conservative estimates in situations where data are incomplete.
- Class I receptors: Use FLM Class I receptor list with receptor elevations provided (available from the NPS).
  - CALPUFF model options: Use IWAQM (EPA, 1998) default guidance, including Pasquill-Gifford dispersion coefficients.
  - Ozone dataset – use observed ozone data for 2001-2003 from CASTNet and AIRS stations. Only non-urban ozone stations should be used in the OZONE.DAT file. Monthly average ozone (backup) background values are to be computed based on daytime average ozone concentrations from the OZONE.DAT file (6am-6pm average ozone concentrations computed by month).
  - Background ammonia concentration: In CALPUFF, use constant (0.5 ppb) value for ammonia.
  - Puff representation: integrated puff sampling methodology.
  - Building downwash: Ignore building downwash unless source is within 50-km of a Class I area and the State instructs the source to specifically consider building downwash.

#### ***CALPOST and POSTUTIL Configuration (Initial exemption modeling)***

- Use Visibility Method 6 in CALPOST
- Species considered in visibility analysis: SO<sub>4</sub>, NO<sub>3</sub>, EC, SOA (i.e., condensable organic emissions), soil, coarse PM
- Natural background light extinction: Several options are acceptable at the discretion of the State: (1) A single annual average natural background extinction for each Class I area, as presented in Appendix B of EPA's natural conditions guidance (EPA, 2003b); (2) A single value that represents the average haze index on the 20% best natural conditions days, again as presented in the same Appendix B; or (3) A monthly average natural background as calculated by CALPOST under Method 6, based on annual average default natural

conditions component concentrations and monthly average  $f(RH)$  values for the centroid of the Class I area, from Table A-3 in the natural conditions guidance document,.

A special procedure is needed for options 1 and 2, since CALPOST requires input of natural background concentrations of PM components while the backgrounds for options 1 and 2 are expressed in EPA's guidance document as extinction coefficients or haze indices (in deciviews). In order to produce the appropriate natural background in CALPOST for these options, use Equation 3-2 to calculate the extinction coefficient that corresponds to EPA's haze index value for the Class I area (if necessary), subtract the Rayleigh scattering value of  $10 \text{ Mm}^{-1}$ , and enter a soil concentration (in  $\mu\text{g}/\text{m}^3$ ) into CALPOST that is numerically equal to this result. (Since the extinction efficiency of soil is  $1 \text{ m}^2/\text{g}$ , Equation 3-1 shows that this process produces a background extinction that equals the EPA's value.) Leave the concentrations of all other species blank, since the number that is entered represents extinction by all components.

- Light extinction efficiencies: Use EPA (2003a) values. If a source chooses, the new IMPROVE algorithm for calculating light extinction (see Section 3.2.3) may be used in addition to the default IMPROVE algorithm. (Calculations would need to be performed outside CALPOST or CALPOST would need to be modified to accommodate the new algorithm.)
- Nitrate repartitioning in POSTUTIL: Do not use for the initial modeling.

The initial run results will be based on the highest change in light extinction (deciviews) from natural conditions over the three-year modeling period for each Class I area considered. Predicted changes exceeding the "contribution" threshold (0.5 deciviews) will trigger a finer grid CALPUFF modeling analysis.

## 4.4 Finer Grid Modeling Procedures

### 4.4.1 Rationale for and Overview of Finer Grid Modeling Approach

There are two potential applications for finer grid CALPUFF modeling:

**BART Exclusion Modeling.** First, finer grid CALPUFF modeling can be used to demonstrate that a source does not cause or contribute to visibility impairment in any Class I areas, and thus can be excluded from BART controls. As shown in Figure 4-1, if the initial regional modeling results are not below the threshold for visibility impacts, the next step is to conduct modeling using a finer grid resolution for the meteorological fields and the treatment of terrain effects and land use variability. In the finer grid modeling the predicted visibility impairment that is compared to the threshold is based on the BART guidance of the 98<sup>th</sup> percentile change in deciviews value rather than the more conservative highest value used in the initial analysis.

The BART guidance indicates that the emissions rate to be used for such modeling is the highest 24-hr rate during the modeling period. Depending on the availability of source data, the following

emissions information (listed in order of priority) should be used with CALPUFF for BART exclusion modeling:

- 24 hr maximum value emissions for the period 2001-2003 (Continuous Emission Monitor, CEM data)
- 24 hr maximum value from continuous emissions monitoring data
- facility stack test emissions
- potential to emit
- permit allowable emissions, if available
- emissions factors from AP-42 source profiles

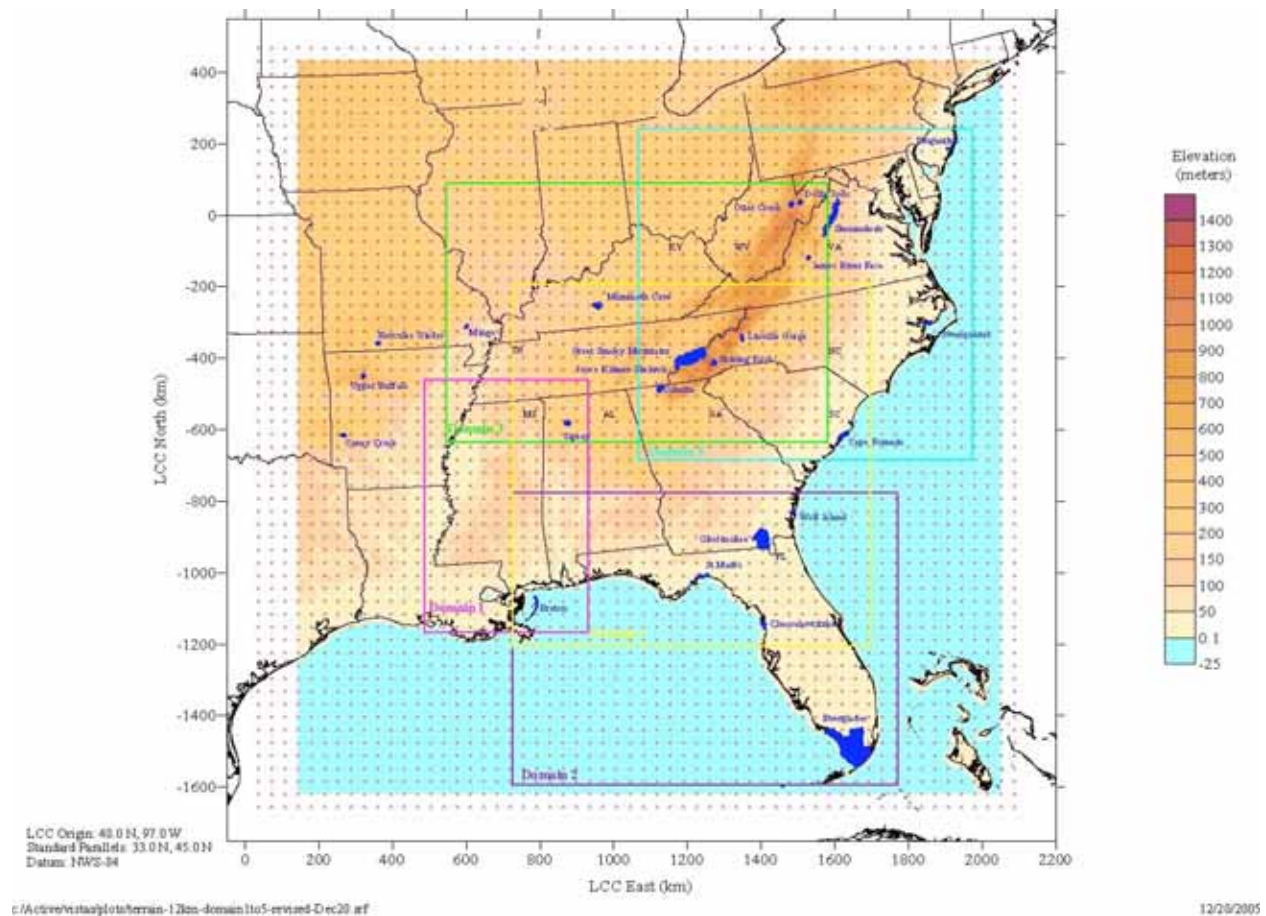
***Quantify Benefits of BART.*** The second application of refined modeling is to quantify the visibility benefits from the BART control options. This is accomplished by running CALPUFF with the baseline emissions rates and again with emissions after BART controls. It is important that emission reductions be evaluated in the postprocessing step rather than by using “negative” emission rates in the CALPUFF model. The chemical scheme requires that emission rates always be positive.

For any of these applications, a source-specific modeling protocol that defines source properties and the specific model configuration is required. As discussed in Section 5, the source specific protocol should include source-specific emissions data and can refer to this document for all methods and assumptions that follow this common protocol.

#### ***4.4.2 Model Configuration and Settings for Finer Grid Modeling***

Grid resolution substantially better than 12-km is needed for a finer grid CALPUFF assessment of visibility impacts in most cases involving Class I areas in complex terrain or coastal areas. Thus, the CALMET fine grid resolution in the subregional modeling domains used for finer grid modeling will depend on the terrain, land use (especially coastal boundaries), location of the source, distance of the source from Class I areas, and total size of the subregional modeling domain.

VISTAS States have 2001-2003 CALMET files for five 4-km sub-regional domains as illustrated in Figure 4-4. The subdomains are designed to address all BART eligible sources within each VISTAS states and all Class I areas within 300 km of the BART-eligible sources. For application for a single source, a smaller domain of roughly 200-300 km by 200-300 km is recommended. Requests to obtain the 4-km CALMET files should be made to the State BART representatives.



**Figure 4-4. The five subregional domains for 4-km CALMET modeling.**

In some instances, as part of the source-specific protocol, a source may propose to the State to use an even finer grid simulation to properly characterize the flow fields and land use changes that affect dispersion. An application for source-receptor distances within about 50 km may require a grid resolution less than 1 km if complex terrain effects are likely to be important. This determination should be made on a case-by-case basis. There is not a single distance at which a particular grid size is appropriate. It depends on factors such as the complexity of the terrain, the source-receptor distances involved, the location of the source relative to the terrain features, the physical stack parameters (e.g., a tall stack in complex terrain may be unaffected by the terrain-forced flow), proximity of the source and Class I area to a coastline, and other factors including availability of representative observational data.

The finer grid CALMET simulations were run in hybrid mode, using both MM5 data to define the initial guess fields and meteorological observational data in the Step 2 calculations. Overwater (buoy) data will be provided in addition to the hourly surface meteorological observations, precipitation observations and twice-daily upper air sounding data.



A domain-specific set of modeling parameters will be defined for each subregional domain. The proper selection of the CALMET diagnostic wind field parameters that are used to blend observations with the Step 1 wind field depends on factors such as the locations of the meteorological stations relative to terrain and coastal features (which affects the representativeness of the observational data), the terrain length scale, and the quality (resolution) of the MM5 data used to define the initial guess field and its ability to properly resolve wind flows on the fine-scale CALMET domain. The definition of the proper CALMET parameters is done as part of sensitivity testing where model performance is evaluated against available observations and expected terrain effects, such as channeling of flows within a valley.

In addition to the better grid resolution and the introduction of observational data in the finer grid simulations, several other modeling refinements can enhance the accuracy of the finer grid modeling. These include use of the higher resolution terrain DEM data (~3 arc sec USGS data) in defining the gridded terrain fields and application of the ammonia limiting method in the POSTUTIL post-processor. Otherwise, the source configuration, emissions, pollutant speciation, Class I receptors, ozone datasets and CALPUFF model options will be the same as in the initial runs. Similarly, CALPOST will be used in the same manner as for the initial analyses. However, POSTUTIL can be used to repartition nitrate in the finer grid modeling, using background ammonia concentrations according to the IWAQM Phase 2 report (IWAQM, 1998).

For the finer grid BART exclusion analysis, the test for evaluating whether a source is contributing to visibility impairment is based on the 98<sup>th</sup> percentile modeled value (rather than the highest predicted value used for the initial evaluation), which is consistent with EPA's BART guidance.

## **4.5 Presentation of Modeling Results**

The CALPOST processing computes the daily maximum change in deciviews. A sample of the summary table produced by CALPOST is shown in Table 4-1. For evaluating compliance with the VISTAS screening threshold, the highest change in extinction value, located at the bottom of the CALPOST list file is compared to the threshold value (e.g., 0.5 dv). For example, in the sample shown in Table 4-1, the summary at the bottom shows that the highest visibility impact is 1.219 dv, with 9 days over the year showing values greater than 0.5 dv. Therefore this source would not pass the initial analysis, and finer grid modeling would be required.

In addition to the highest change in deciview value on each day over all the receptors in a particular Class I area, the CALPOST summary table in Table 4-1 contains the coordinates of the receptor, receptor type (D indicates discrete receptors), the total haze level (background + source, in dv), the background haze in deciviews, the change in haziness (delta dv), the humidity term applied to hygroscopic aerosols (f(RH)), and the contribution of each species to light extinction (in percent of the total source contribution) for SO<sub>4</sub>, NO<sub>3</sub>, organics, elemental carbon, coarse and fine particulate matter.

**Table 4-1. Example of CALPOST Output, Showing Maximum Daily Impacts of Source and Locations of Those Impacts.**

YEAR	DAY	HR	RECEPTOR	COORDINATES (km)		TYPE	DV(Total)	DV(BKG)	DELTA	DV	F(RH)	%_SO4	%_NO3	%_OC	%_EC	%_PMC	%_PMF
2001	2	0	3	20.540	79.782	D	5.397	5.358	0.039	4.314	44.33	47.22	3.07	1.07	0.00	4.30	
2001	3	0	9	31.680	79.822	D	4.566	4.421	0.145	1.767	40.75	33.89	9.19	3.24	0.00	12.94	
2001	4	0	1	24.723	77.951	D	4.540	4.540	0.000	2.076	0.00	0.00	0.00	0.00	0.00	0.00	
2001	5	0	77	30.228	94.571	D	4.950	4.939	0.011	3.144	43.13	44.74	4.64	1.45	0.00	6.05	
2001	6	0	1	24.723	77.951	D	5.181	5.166	0.015	3.772	38.58	56.05	1.90	0.70	0.00	2.76	
2001	7	0	3	20.540	79.782	D	6.366	5.745	0.620	5.439	44.98	44.99	3.69	1.26	0.00	5.08	
.																	
.																	
.																	
2001	363	0	113	27.414	103.782	D	5.725	5.652	0.073	5.164	53.49	35.51	4.03	1.39	0.00	5.58	
2001	364	0	113	27.414	103.782	D	6.554	6.521	0.033	7.826	48.12	47.09	1.67	0.64	0.00	2.48	
2001	365	0	1	24.723	77.951	D	6.499	6.499	0.000	7.757	0.00	0.00	0.00	0.00	0.00	0.00	
--- Number of days with Delta-Deciview =>						0.50:	9										
--- Number of days with Delta-Deciview =>						1.00:	2										
---						Largest Delta-Deciview =	1.219										

For the finer grid analysis, the data in the table can be imported into a spreadsheet and sorted on the delta dv column. Table 4-2 shows an example of the ranked visibility impacts (change in dv) for each of three years at six different Class I areas. The 98<sup>th</sup> percentile (8<sup>th</sup> highest value) in the sorted table would be compared to the contribution threshold (e.g., 0.5 dv). In the example shown in this table, the source passes the finer grid analysis because the highest 98<sup>th</sup> percentile visibility impact is below the contribution threshold of 0.5 dv.

The Results section of the CALPUFF modeling report should contain the following information:

1. Map of source location and Class I areas within 300 km of the source
2. For the VISTAS 12-km CALPUFF initial exemption modeling domain, a table listing all Class I areas in the VISTAS domain and those in neighboring states and impacts at those Class I areas within 300 km of the source, as illustrated in Table 4-3.
3. A discussion of the number of Class I areas with visibility impairment from the source on 98<sup>th</sup> percentile days in each year greater than 0.5 dv (total visibility impairment minus impairment on 20% best days for natural background visibility equals delta-dv, the visibility impact attributed to the source).
4. For the Class I area with the maximum impact, discussion of the number of days below the 98<sup>th</sup> percentile that the impact of the source exceeds 0.5 dv, the number of receptors in the Class I area where the impact exceeds 0.5 dv, and the maximum impact.
5. For finer grid CALPUFF exemption modeling, results for those Class I areas for which impacts of the source exceeded 0.5 dv in the 12-km initial exemption modeling. Report same results as provided for 12-km initial exemption modeling.
6. For control option modeling, each control option tested should be listed in tabular format. For each control option and for each Class I area where the impact of the source exceeded 0.5 dv, report the change in pollutant emissions and the change in visibility impact from the source as a result of the control option. The effectiveness of candidate control options are to be compared to each other, not to a specific target improvement.

States will provide further guidance on graphic presentation of results to simplify evaluation of effectiveness of control measures. For example, a temporal plot of the change in deciviews between the controlled and uncontrolled cases could be developed for the receptor with the maximum modeled impact in each Class I area.

7. Copies of all input files and input data in electronic format for the CALMET, CALPUFF, CALPOST and POSTUTIL runs should be archived and provided to the State.

**Table 4-2. Example of Visibility Impact Rankings at Six Class I Areas**

Class I Area	2001	2002	2003
	Delta- Deciview Ranks 1-8	Delta- Deciview Ranks 1-8	Delta- Deciview Ranks 1-8
Great Smoky NP	0.99	0.95	1.20
	0.88	0.63	0.90
	0.62	0.51	0.73
	0.59	0.50	0.72
	0.55	0.46	0.59
	0.52	0.42	0.47
	0.48	0.37	0.45
	0.47	0.36	0.42
Linville Gorge	0.67	0.81	0.76
	0.45	0.69	0.47
	0.43	0.65	0.37
	0.33	0.50	0.35
	0.29	0.45	0.31
	0.27	0.33	0.30
	0.25	0.31	0.28
	0.23	0.29	0.28
Shining Rock	0.66	0.73	0.75
	0.43	0.69	0.45
	0.41	0.63	0.36
	0.35	0.52	0.34
	0.26	0.46	0.28
	0.24	0.34	0.27
	0.23	0.29	0.26
	0.22	0.26	0.25
Cohutta	0.26	0.54	0.61
	0.23	0.47	0.42
	0.22	0.43	0.30
	0.21	0.37	0.29
	0.20	0.37	0.28
	0.19	0.31	0.28
	0.18	0.31	0.25
	0.16	0.30	0.25
Joyce Kilmer-Slickrock	0.34	0.52	0.27
	0.33	0.43	0.24
	0.31	0.32	0.23
	0.26	0.31	0.20
	0.24	0.30	0.14
	0.20	0.28	0.13
	0.18	0.24	0.11
	0.17	0.24	0.10
Mammoth Cave NP	0.56	0.57	0.50
	0.44	0.56	0.37
	0.38	0.53	0.36
	0.29	0.35	0.35
	0.25	0.33	0.31
	0.24	0.33	0.24
	0.22	0.30	0.21
	0.21	0.29	0.19

**Table 4-3. Format of Summary of Results for CALPUFF Modeling in VISTAS' 12-km Modeling Domain to Determine if a BART Eligible Source is Subject to BART.**

Class I area	Distance (km) from source to Class I area boundary	# of days <sup>1</sup> and # of receptors with impact > 0.5 dv in Class I area: 2001		# of days <sup>1</sup> and # of receptors with impact > 0.5 dv in Class I area: 2002		# of days <sup>1</sup> and # of receptors with impact > 0.5 dv in Class I area: 2003		# of days <sup>1</sup> and # of receptors with impact > 1.0 dv in Class I area for 3-yr period		Max. 24-hr impact over 3-yr period
Dolly Sods, WV										
Shenandoah, VA										
James River Face, VA										
Mammoth Cave, KY										
Sipsey, AL										
Great Smoky Mtns, TN										
Cohutta, GA										
Shining Rock, NC										
Linville Gorge, NC										
Swanquarter, NC										
Cape Romain, SC										
Okefenokee, GA										
Saint Marks, FL										
Chassahowitzka, FL										
Everglades, FL										
Brigantine, NJ										
Breton Island, LA										
Caney Creek, AR										
Upper Buffalo, AR										
Mingo, MO										
Hercules Glade, MO										

<sup>1</sup>Days below the 98<sup>th</sup> percentile of days in each year or the three-year modeling period, as appropriate

## 4.6 VISTAS Contribution to CALPUFF Modeling of BART Eligible Sources

VISTAS will provide updates and supporting information concerning the Common Modeling Protocol (this document) on the VISTAS website. In addition, VISTAS will make publicly available the following data bases developed by Earth Tech:

- VISTAS version of the CALPUFF modeling system, maintained on the CALPUFF website. Version 5.754 includes CALMET, CALPUFF, CALPOST, and POSTUTIL files, updated in December 2005. The last update in this VISTAS version is a CALMET update that addresses over water dispersion, which was developed for the Minerals Management Service (MMS) in fall 2005. This VISTAS version of CALPUFF will not be updated further unless errors are found in the code, except that a new one-step POSTUTIL procedure will be incorporated. BART-eligible sources in the VISTAS states will be able to use this VISTAS version throughout the BART modeling exercise.
- 12-km CALMET output files for 2001, 2002, and 2003 produced as described in previous sections. Further detail on model configuration and settings will be provided with the output files and will be made available on the CALPUFF website.
- CALMET will include a software modification to allow the meteorological data inputs into CALMET to be used to generate finer grid CALMET files without having to go back to the original MM5 output files
- Five 4-km CALMET subdomains for 2001, 2002, and 2003, produced as described in previous sections. Further detail on model configuration and settings will be provided with the output files and will be made available on the website.
- File with CALPUFF model configuration and settings sufficient to replicate CALPUFF modeling done for VISTAS using 12 km CALMET, including
  - Ozone data used to run CALPUFF
  - Ammonia concentrations used to run CALPUFF.
  - All other set up files used in VISTAS 12-km CALPUFF run

Samples of these data files and examples of their application with CALPUFF for BART screening analyses can be found on the CALPUFF web site at ([http://www.src.com/verio/download/sample\\_files.htm](http://www.src.com/verio/download/sample_files.htm)).

## 5. SOURCE-SPECIFIC MODELING PROTOCOL

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Sources are required to submit a source-specific protocol to the State for review and approval prior to source-specific modeling. States will provide the documentation to EPA and FLM for their review. An outline of the typical contents of the site-specific protocol is provided in Table 5-1.

If a source-specific modeling approach is proposed that differs from the common approach in Chapter 4, a more-detailed modeling protocol than that required under the common procedures is required. This protocol must explain the data sources, model configuration, and rationale for changes in the model approach from the common protocol and must be approved by the State.

Unit-specific source data include the following parameters:

- Location (e.g., UTM coordinates, UTM zone and datum)
- Stack height above the ground
- Stack diameter
- Exit velocity
- Exit temperature
- Emission rates ( $\text{SO}_2$ ,  $\text{H}_2\text{SO}_4$ ,  $\text{NO}_x$  and  $\text{PM}_{10}$ ).

Additional building dimension information (building width, length, height and corner locations) is needed for short stacks that are less than Good Engineering Practice (GEP) height. This information is used in providing effective structure dimensions for building downwash calculations. (The requirement to conduct building downwash modeling may be waived by individual States or if the transport distance is greater than 50 km.)

The source coordinates must be expressed in the coordinate system used to define the CALMET and CALPUFF modeling domains. For the regional screening simulations, a Lambert Conformal Conic (LCC) coordinate system will be used. The required parameters to define an LCC coordinate include two matching parallels, latitude/longitude of the projection origin, coordinate datum, and false Easting and Northing (if used) of the projection origin. Subregional and source-specific domains may be using either an LCC or UTM projection.

The CALPUFF Graphical User Interface (GUI) system provides software (called COORDS) to compute to/from latitude/longitude, LCC and UTM coordinates for a large number of datums. In addition, the CALVIEW graphics feature allows the use of georeferenced satellite or aerial photographs to be used as base maps to confirm source locations. Links to sources of suitable base maps can be found on the CALPUFF data site ([www.src.com](http://www.src.com)) in the section on “Aerial Photos”.

**Table 5-1. Sample Table of Contents of a Source-Specific Fine-Scale Modeling Protocol.**

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1.	INTRODUCTION
1.1	Objectives
1.2	Location of Source vs. Relevant Class I Areas
1.3	Source Impact Evaluation Criteria
2.	SOURCE DESCRIPTION
2.1	Unit-specific Source Data
2.2	Boundary Conditions
3.	GEOPHYSICAL AND METEOROLOGICAL DATA
3.1	Modeling Domain and Terrain
3.2	Land Use
3.3	Meteorological Data Base
3.3.1	MM5 Simulations
3.3.2	Measurements and Observations
3.4	Air Quality Data Base
3.4.1	Ozone Concentrations – Measured or Modeled
3.4.2	Ammonia Concentrations – Measured or Modeled
3.4.3	Concentrations of Other Pollutants – Measured or Modeled
3.5	Natural Conditions at Class I Areas
4.	AIR QUALITY MODELING METHODOLOGY
4.1	Plume Model Selection
4.1.1	Major Relevant Features of CALMET
4.2.2	Major Relevant Features of CALPUFF
4.2	Modeling Domain Configuration
4.3	CALMET Meteorological Modeling
4.4	CALPUFF Computational Domain and Receptors
4.5	CALPUFF Modeling Option Selections
4.6	Light Extinction and Haze Impact Calculations
4.7	Modeling Products
5.	REVIEW PROCESS
6.1	CALMET Fields
6.2	CALPUFF, CALPOST, and POSTUTIL Results
6.	REFERENCES
	APPENDICES
A.1	VISTAS BART MODELING PROTOCOL
A.2	... other appendices as needed



An example of the data that need to be reported is provided in Table 5-2. More detail on the stack data, emissions species, and particulate size fractions to be reported will be made available on the CALPUFF website, [www.src.com](http://www.src.com). Check with your State for the more detailed format of Table 5-2 that is to be used.

Discussions with the regulatory authorities should be conducted prior to development of a protocol to ensure all of the relevant issues are included in the protocol.

**Table 5-2. Example of Source Documentation for BART Eligible Source.**

<b>Unit name and/or description</b>	<b>Start-up dates</b>	<b>SO<sub>2</sub> potential emissions (tpy)</b>	<b>NO<sub>x</sub> potential emissions (tpy)</b>	<b>Total PM potential emissions (tpy)</b>
Emissions source name				
...				
Total emissions				
Potential BART-eligible emissions				

## **6. QUALITY ASSURANCE**

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### **6.1 Scope and Purpose of the QA program**

Air quality modeling covered under this protocol is an important tool for use in determining whether a BART-eligible source can be reasonably expected to cause or contribute to visibility impairment in a Class I area, and therefore whether this source should be subject to BART controls, and if so, to determine the relative benefits of various BART controls. The purpose of the quality assurance (QA) program is to establish procedures for ensuring that products produced by the application of the modeling techniques for BART studies satisfy the regulatory objectives of the BART program.

The scope of the QA program affects different users differently. Common features of most applications will be the setup and execution of the CALPUFF air quality model and processing of modeling results to determine if a source contributes to visibility impairment at a Class I area. In many cases, users will be provided meteorological datasets that have been developed with VISTAS funding under a suitable QA program for use in the BART modeling. Other users will be involved in site-specific or source-specific analyses that will use additional datasets and potentially different modeling options and/or tools. More extensive quality assurance will be required in these latter types of applications. It is the responsibility of the modeler to ensure that an adequate QA protocol is in place for a particular application.

The CALPUFF modeling system contains built-in features to facilitate quality assurance of the modeling results. These include the automatic production of “QA” files for various datasets, including geophysical fields, sources and receptors, and imbedded tracking of model options and switches within the output files from the major modeling units of the modeling system. The Graphical User Interface system (GUI) provided as part of the latest CALPUFF modeling system allows these QA files to be displayed graphically.

In addition, a detailed software management system is in place to track version and level numbers associated each program and utility within the CALPUFF modeling system. This information is carried forward in all of the output files to create an audit trail of software versions and major model options used that can be retrieved and displayed from the model output files.

Because the required QA procedures will depend heavily on the exact application, there will be differences among different users and different applications.

In addition, the BART modeling process involves multiple organizations. The States have overall responsibility for the process and may also execute some or all of the modeling. VISTAS is contributing general guidance via this protocol and is preparing meteorological fields and performing modeling under the guidance of the States. The sources that are BART-eligible need to provide process information and emissions data for use in the analyses. In addition, those sources that are involved in BART assessments will need to be actively involved in control

technology decisions and assessments. Finally, some of the modeling steps may be carried out by contractors on behalf of VISTAS, a State, or a source.

Each of these organizations has a responsibility to ensure that it is providing correct information to others and to evaluate the quality of any analyses it is performing, whether with data of its own or from others. This chapter provides general guidance and information on those aspects of quality assurance that are specific to the CALPUFF modeling effort, irrespective of which organization is carrying out the effort. The focus is on the common protocol efforts described in Chapter 4. As described in Section 6.3, more comprehensive QA may be needed for the unique aspects of the source-specific modeling described in Chapter 5.

## **6.2 QA Procedures for Common Protocol Modeling**

The VISTAS common protocol (Section 4) describes the methods and procedures for use in conducting regional scale screening modeling to determine whether a particular source or group of sources is subject to BART controls. In the initial application, the regional CALPUFF-ready meteorological data files will be provided by VISTAS. The amount of effort for end-users performing QA of these pre-defined meteorological fields will be reduced from what is required in developing source-specific meteorological fields, as described below. Also, VISTAS is planning to provide five subregional CALMET meteorological datasets in a CALPUFF-ready format. The development of these CALMET datasets will be subject to a QA program as part of their development, so the necessary quality assurance activity of end-users is again reduced from what would be required in the development of the dataset. It is not expected that the quality assurance steps in the development will be repeated in each application. The VISTAS-provided regional and subregional meteorological fields will include a test case simulation for demonstrating that expected modeling results are obtained on the user's computer platform. This test should be repeated by every user.

Although the CALPUFF modeling system is recommended by the U.S. Environmental Protection Agency for application to BART analyses, a considerable amount of expertise and modeling judgment is needed at certain stages of the analysis. The modeling is not a "cookbook" exercise, a fact that was recognized by the U.S. EPA in describing the expertise needed for CALMET modeling (EPA, 1998; pp. 9-10,). Current methods for performing refined chemistry calculation also require an understanding of the chemical and meteorological processing affecting ammonium nitrate formation. VISTAS has committed to provide appropriate CALPUFF training to assist States in obtaining the necessary expertise with the latest CALPUFF modeling tools and techniques. An appropriate level of knowledge of the model formulation, technical approach and assumptions is essential for successful BART modeling.

### ***6.2.1 Quality Control of Input Data***

The input data required by the model depends on the application. At a minimum, source data is required by CALPUFF (see Section 6.2.3) along with a list of choices made about model options and switches. Most of the modeling option choices are specified or recommended by regulatory

guidance and default values (see references in Section 4.3.3). However, remodeling of the boundary conditions is not required for VISTAS-provided finer grid domains so the expertise level is not as high as it would be for development of the boundary conditions files from scratch.

To the extent that modeling applications are using pre-defined CALMET files and CALPUFF templates, the quality assurance will be straightforward. More detailed steps are needed for the setup of modeling files for source-specific applications of subregional domains finer than 4 km.

The basic procedures that will apply to all CALPUFF model applications will include a confirmation of the source data, including units, verification of the correct source and receptor locations, including datum and projection, confirmation of the switch selections relative to modeling guidance, checks of the program switches and file names for the various processing steps, and confirmation of the use of the proper version and level of each model program. It is a common and recommended procedure for an independent modeler not involved in the setup of the modeling files to independently confirm the model switches and data entry in the actual model input files and to conduct an independent run of the worst case event as a confirmation check.

In addition, common practice requires that a model project CD (or DVD or set of DVDs) be created that contains all of the data and program files needed to reproduce the model results presented in a report. The model list files from each step are included on the project CD. This information allows independent checking and confirmation of the modeling process.

### ***6.2.2 Quality Control of Application of CALMET***

For users of the VISTAS CALPUFF-ready CALMET meteorological files, a number of large datafiles will be provided by VISTAS on external USB2 or Firewire hard drives in a format ready for use with the CALPUFF model. The QA steps associated with the development of the VISTAS common datasets will be provided separately as part of the modeling documentation. It is not expected that the QA steps conducted in the development of the meteorological datasets will be repeated in each application, although tests to confirm that the dataset is suitable for the application for which it is being used should be performed as part of the QA. This is discussed in more detail below.

The regional screening CALMET grid is defined in Chapter 4 on a 12-km Lambert Conformal Conic (LCC) grid system. The subregional and source-specific domains may be defined in either LCC or Universal Transverse Mercator (UTM) coordinates. In the case of the LCC projection, two matching parallels, latitude/longitude of the projection origin, coordinate datum, and false Easting and Northing (if used) of the projection origin must also be defined. For any domains in UTM coordinates, the UTM zone (see Appendix D of the CALMET User's Guide) and datum must be defined. The appropriate projection and map factors are provided as part of the definition of the VISTAS regional grid system. For a source-specific domain, the grid parameters will be provided as part of the source-specific protocol.

Appendix A of the IWAQM report (EPA, 1998) contains a list of recommended CALMET switch settings. Except as modified in Chapter 4 of this protocol or in a source-specific protocol, the IWAQM guidance should be used in setting up the CALMET simulations. The CALMET model obtains the switch settings from an ASCII “control file” with a default name of CALMET.INP. Whether the model is run using a GUI or from the control line in a DOS, Linux, or Unix window, it is essential that the control file be reviewed as part of the CALMET QA analysis. The CALMET GUI retains all of the input descriptive information that is part of the standard CALPUFF.INP file structure. This includes the default value for each variable, a text description of the variable, the meaning of each variable option, the units of the variable and inter-relationships among variables indicating if/when the variable is used. Some third-party commercial GUIs strip out this descriptive information, which makes the QA step more difficult, although it is essential to perform nonetheless using the variable names as references for the variables in the file.

Part of the CALPUFF modeling system’s built-in QA capabilities is a variable tracking system that retains the control file inputs for CALMET and CALPUFF in the output files created by the models. This information includes the Version and Level numbers of the processor codes and main model codes used in the simulations as well as the control files from the main models (CALMET and CALPUFF). The information from the preprocessing steps and the CALMET and CALPUFF model simulations is all carried forward and saved in the CALPUFF/postprocessor output files so that the final concentration/flux files contain a history of the model options and switch settings. This allows a user or reviewing agency to confirm the switch settings provided in a control file with that actually used in the model simulations. An optional switch in the CALPOST processor creates a complete listing of the QA data. This step requires access to the output CALPUFF concentration and/or flux files, which are normally practical to store on CDs or DVDs and to provide a part of the Project CD/DVD set.

### ***6.2.3 Quality Control of Application of CALPUFF***

The quality assurance of the source and emissions data is a major component of the CALPUFF modeling. Also, many errors are found in source coordinates and related projection/datum parameters, so confirmation of the source location is an important part of the modeling QA.

The locations of the Class I area receptors are another important CALPUFF input. The use of pre-defined receptors as provided by the National Park Service (NPS) receptor dataset is recommended in the VISTAS common protocol. However, although the latitude and longitude of each receptor point is provided, it is necessary to ensure that the proper UTM or LCC coordinates have been computed for computational domain selected. In particular, the datum of the NPS conversion software is not specified, so it is recommended that coordinates be checked using the CALPUFF GUI’s COORDS software or another comparable coordinate translation software package that recognizes various datums.

Most of the CALPUFF input variables contain default values. Appendix B of the IWAQM report contains a list of recommended CALPUFF switch settings. Except as modified in Chapter 4 of

this protocol or in a source-specific protocol, the IWAQM guidance should be used in setting up the CALPUFF simulations. The CALPUFF model obtains the switch settings from an ASCII “control file” with a default name called the CALPUFF.INP file. As is the case with the comparable CALMET file, it is essential that the control file be reviewed manually as part of the CALPUFF QA analysis. To facilitate this process, as was the case with the CALMET GUI, the CALPUFF GUI retains all of the input descriptive information that is part of the standard CALPUFF.INP file structure. Some third-party commercial GUIs strip out this descriptive information, which makes the QA step more difficult, although it is essential for perform nonetheless using the variable names as references for the variables in the file.

#### ***6.2.4 Quality Control of Application of CALPOST and POSTUTIL***

CALPOST is run separately for each Class I area in order to obtain the necessary visibility statistics for evaluating compliance with the BART screening and finer grid modeling thresholds. The inputs to CALPOST involve selection of the visibility method (Method 6 in the standard EPA BART guidance), entry of Class I area-specific data for computing background extinction (either average or best 20% natural conditions, as prescribed by the State) and monthly relative humidity factors for hygroscopic aerosols. CALPOST contains a receptor screening that allow subsets of a receptor network modeling in CALPUFF to be selected for processing in a given CALPOST run. This is how receptors within a single Class I area are selected for processing from a CALPUFF output file that may contain receptors from several Class I areas. CALPOST contains options for creating plot files that will help in the confirmation that the proper receptor subset is extracted.

The CALPOST output file contains a listing of the highest visibility impact each day of the model simulation over all receptors included in CALPOST analysis. Receptors will normally be selected in each CALPOST run so that each CALPOST run represents the impacts at a single Class I area. The table includes the data shown in the example in Table 4-1. For a screening assessment, the peak value of the change in extinction is shown at the bottom of the visibility table (see Table 4-1). For a finer grid simulation, the 98<sup>th</sup> percentile value (8<sup>th</sup> highest day) is used for comparison against the BART threshold of 0.5 deciviews. It is necessary to import the results of the CALPOST table into a sorting program such as a spreadsheet to rank the daily change in extinction values such as is presented in Table 4-2.

The CALPOST inputs that need to be carefully checked as part of the CALPOST quality assurance are:

- Visibility technique (Method 6 in the common VISTAS protocol)
- Monthly Class I-specific relative humidity factors for Method 6
- Background light extinction values

- Inclusion of all appropriate species from modeled sources (e.g., sulfate, nitrate, organics, (as SOA), coarse and fine particulate matter and elemental carbon.
- Appropriate species names for coarse PM used
- Extinction efficiencies for each species
- Appropriate Rayleigh scattering term ( $10 \text{ Mm}^{-1}$  for screening modeling but Class I area specific value for finer grid modeling)
- Screen to select appropriate Class I receptors for each CALPOST simulation.

The CALPOST program produces plot files compatible with CALVIEW that allow confirmation of receptor locations that is useful in evaluating the receptor screening step.

POSTUTIL allows the user to sum the contributions of sources from different CALPUFF simulations into a total concentration file. In addition, it contains options to scale the concentrations from different modeled species (e.g., different particle sizes) into species-dependent size distributions for the particulate matter. For example, PM is often simulated with unit emission rates for each particle size category and, in the POSTUTIL stage, the contributions of each size category based on the species being considered (e.g., elemental carbon, coarse particulate matter, etc.) are combined to form the species concentrations for input into CALPOST. This process, although simple, requires a careful review of the weighting factors for each source. POSTUTIL also allows a repartitioning of nitric acid and nitrate to account for the effects of ammonia limiting conditions.

If source-specific modeling is performed using different sources of data or different techniques, the source-specific modeling protocol should provide justification for deviations from the VISTAS common protocol, and a QA plan specific for the application provided to address the quality assurance of the data used.

### **6.3 Additional QA Issues for Alternative Source-Specific Modeling**

The level of QA required for application of source-specific protocols will be substantially higher than for the use of datasets that have already been subject to a QA procedure. For example, source-specific protocols may include the use of on-site meteorological datasets, the use of higher resolution prognostic meteorological (e.g., MM5) datasets, alternative visibility calculations, different extinction coefficients, or other changes to the common protocol. In addition to providing a source-specific modeling protocol describing and justifying the changes to the modeling approach from the VISTAS common protocol, the site-specific applications should include the development of a QA plan to properly evaluate the data used in the site-specific modeling.

The critical CALMET input parameters depend on the mode in which the model is run (observations mode, hybrid mode or no-observations mode), and the location and spatial

representativeness of any observational data. In a site specific protocol involving the development of a meteorological dataset, the elements of the QA process include preparation of wind rose (using observed, MM5 and CALMET-derived data), including examination of the data as a function of season and time of day (e.g., 4am, 10am, 4pm wind roses), time series analyses, and presentation of 2-D vector plots illustrating terrain effects/sea breeze circulation or other features of the flow expected to occur within the domain. For example, 2-D vector plots produced during light wind speed stable conditions (e.g., early morning such as 4 am) are good for assessing the performance of the CALMET model configuration and switches in reproducing terrain effects because these conditions are likely to maximize the terrain impacts in the model. Season wind roses at 4 am, 10 am and 4 pm would be expected to show the development of sea breeze circulations that may be important for certain applications. Customization of the QA process for the individual site-specific domain based on the availability of data and the physical processes expected to be important at that location should be conducted as part of the site-specific QA plan development.

If site-specific CALPUFF simulations involving the Ammonia Limiting Method are conducted, performance of the model in reproducing observed CASTNet or IMPROVE sulfate and nitrate concentrations at measurement sites within the site-specific modeling domain should be evaluated. The use of alternative ammonia concentration data (e.g., CMAQ output rather than derived ammonia based on aerosol measurements) will require an evaluation of the model performance relative to the techniques in the VISTAS common protocol.

In any site-specific protocol a site-specific QA plan should be prepared.

## **6.4 Assessment of Uncertainty in Modeling Results**

Chapter 3 discussed the uncertainties and known limitations in CALPUFF. The source specific modeling report does not need to repeat the uncertainties listed in Chapter 3, but the reviewer should interpret results in light of these limitations. It is expected that the performance of the model will be better in predicting changes in visibility impacts due to BART controls than in predicting absolute visibility values. This is because uncertainties in meteorological conditions transport and dispersion are expected to be less important in evaluating a change in impact, since a comparable effect will be included in both the base and sensitivity simulations.



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